

This Page Is Inserted by IFW Operations  
and is not a part of the Official Record

## **BEST AVAILABLE IMAGES**

Defective images within this document are accurate representations of the original documents submitted by the applicant.

Defects in the images may include (but are not limited to):

- BLACK BORDERS
- TEXT CUT OFF AT TOP, BOTTOM OR SIDES
- FADED TEXT
- ILLEGIBLE TEXT
- SKEWED/SLANTED IMAGES
- COLORED PHOTOS
- BLACK OR VERY BLACK AND WHITE DARK PHOTOS
- GRAY SCALE DOCUMENTS

**IMAGES ARE BEST AVAILABLE COPY.**

**As rescanning documents *will not* correct images,  
please do not report the images to the  
Image Problem Mailbox.**

**PCT**WORLD INTELLECTUAL PROPERTY ORGANIZATION  
International Bureau

## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification <sup>6</sup> : <b>C12N 9/16, C12P 21/06</b>		A2	(11) International Publication Number: <b>WO 97/06246</b> (43) International Publication Date: 20 February 1997 (20.02.97)
(21) International Application Number: <b>PCT/US96/12818</b>			(81) Designated States: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, ARIPO patent (KE, LS, MW, SD, SZ, UG), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).
(22) International Filing Date: 1 August 1996 (01.08.96)			
(30) Priority Data: 08/512,815 9 August 1995 (09.08.95) US			
(71) Applicant: VERTEX PHARMACEUTICALS INCORPORATED [US/US]; 130 Waverly Street, Cambridge, MA 02139-4242 (US).			
(72) Inventors: ARMISTEAD, David, M.; Five Cutting Drive, Maynard, MA 01754 (US). FITZGIBBON, Matthew, James; 163 Exchange Street, Millis, MA 02054 (US). FLEMING, Mark, Andrew; 413 Cardinal Medeiros Avenue, Cambridge, MA 02141 (US). GRIFFITH, James, P.; 15 Wood Ridge Circle, Weston, MA 02193 (US). KIM, Eunice, E.; 1500 Worcester Road, Framingham, MA 01701 (US). KIM, Joseph, L.; 20 Ridge Avenue, Natick, MA 01760 (US). SINTCHAK, Michael, D.; 34 Lloyd Street, Winchester, MA 01890 (US). THOMSON, John, Allan; 105 Slade Street, Belmont, MA 02178 (US). WILSON, Keith, P.; 6 Longwood Drive, Hopkinton, MA 01748 (US).			Published <i>Without international search report and to be republished upon receipt of that report.</i>
(74) Agents: HALEY, James, F., Jr. et al.; Fish & Neave, 1251 Avenue of the Americas, New York, NY 10020-1104 (US).			
(54) Title: MOLECULES COMPRISING A CALCINEURIN-LIKE BINDING POCKET AND ENCODED DATA STORAGE MEDIUM CAPABLE OF GRAPHICALLY DISPLAYING THEM			
(57) Abstract			
<p>The present invention relates to crystallized molecules and molecular complexes which comprise the active site binding pocket or the FKBP12/FK506 binding pocket of calcineurin or close structural homologues to either binding pocket. This invention also relates to a data storage material encoded with the corresponding structure coordinates of those crystallized molecules or molecular complexes. Such data storage material is capable of displaying such molecules and molecular complexes as a graphical three-dimensional representation on a computer screen. In addition, this invention relates to methods of using the structure coordinates of those molecules or molecular complexes to solve the structure of homologous proteins. This invention also relates to methods of using the structure coordinates to screen and design compounds that bind to calcineurin or homologues thereof.</p>			

**FOR THE PURPOSES OF INFORMATION ONLY**

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AM	Armenia	GB	United Kingdom	MW	Malawi
AT	Austria	GE	Georgia	MX	Mexico
AU	Australia	GN	Guinea	NE	Niger
BB	Barbados	GR	Greece	NL	Netherlands
BE	Belgium	HU	Hungary	NO	Norway
BF	Burkina Faso	IE	Ireland	NZ	New Zealand
BG	Bulgaria	IT	Italy	PL	Poland
BJ	Benin	JP	Japan	PT	Portugal
BR	Brazil	KE	Kenya	RO	Romania
BY	Belarus	KG	Kyrgyzstan	RU	Russian Federation
CA	Canada	KP	Democratic People's Republic of Korea	SD	Sudan
CF	Central African Republic	KR	Republic of Korea	SE	Sweden
CG	Congo	KZ	Kazakhstan	SG	Singapore
CH	Switzerland	LI	Liechtenstein	SI	Slovenia
CI	Côte d'Ivoire	LK	Sri Lanka	SK	Slovakia
CM	Cameroon	LR	Liberia	SN	Senegal
CN	China	LT	Lithuania	SZ	Swaziland
CS	Czechoslovakia	LU	Luxembourg	TD	Chad
CZ	Czech Republic	LV	Latvia	TG	Togo
DE	Germany	MC	Monaco	TJ	Tajikistan
DK	Denmark	MD	Republic of Moldova	TT	Trinidad and Tobago
EE	Estonia	MG	Madagascar	UA	Ukraine
ES	Spain	ML	Mali	UG	Uganda
FI	Finland	MN	Mongolia	US	United States of America
FR	France	MR	Mauritania	UZ	Uzbekistan
GA	Gabon			VN	Viet Nam

MOLECULES COMPRISING A CALCINEURIN-LIKE  
BINDING POCKET AND ENCODED DATA STORAGE  
MEDIUM CAPABLE OF GRAPHICALLY DISPLAYING THEM

TECHNICAL FIELD OF INVENTION

5           The present invention relates to crystallized molecules and molecular complexes which comprise the active site binding pocket or the FKBP12/FK506 binding pocket of calcineurin or close structural homologues to either binding pocket. This invention also relates to a  
10          data storage medium encoded with the corresponding structure coordinates of those crystallized molecules or molecular complexes. Such data storage material is capable of displaying such molecules and molecular complexes as a graphical three-dimensional representation  
15          on a computer screen. In addition, this invention relates to methods of using the structure coordinates of those molecules or molecular complexes to solve the structure of homologous proteins. This invention also relates to methods of using the structure coordinates to  
20          screen and design compounds that bind to calcineurin or homologues thereof.

BACKGROUND OF THE INVENTION

FK506 is an immunosuppressant that inhibits T-cell activation and proliferation [B. E. Bierer et al.,  
25          Current Opinions in Immunology, 5, pp. 763-773 (1993)].  
Immunosuppressants, such as FK506, are useful drugs in

the treatment of transplant rejection and the prevention of autoimmune diseases. Furthermore, such compounds are useful tools in immune system research.

5 FK506 is a more recently discovered and more potent immunosuppressant than cyclosporin.

Unfortunately, FK506 is characterized by undesirable pharmacological properties, such as toxicity and poor bioavailability [P. Neuhaus et al., Lancet, 344, pp. 423-428 (1994)]. Therefore, there remains a need for potent 10 immunosuppressants with improved pharmacological properties.

15 FK506 acts as an immunosuppressant by inhibiting T-cell signal transduction pathways that control lymphokine transcription factors. As a result, gene activation of various lymphokines, including IL-2, is prevented. This in turn leads to an inhibition of T-cells, and therefore, immunosuppression.

20 FK506 exerts these effects in a step-wise process. Initially, FK506 binds to a peptidyl prolyl isomerase, FK506 Binding Protein ("FKBP12"). This complex then binds to, and inhibits, calcineurin. Subsequent events inhibit signal transduction pathways, inhibit lymphokine gene transcription, and ultimately, reduce production of lymphokines, such as IL-2.

25 Calcineurin is a  $\text{Ca}^{2+}$ -dependent serine/threonine phosphatase. It is a heterodimer composed of 2 subunits: calcineurin A ("CnA"), a 59kDa catalytic subunit and calcineurin B ("CnB"), a 19kDa subunit. CnA contains a phosphatase active site and an autoinhibitory region as well as binding sites for calmodulin and CnB. Binding of 30 FKBP12/FK506 inhibits the phosphatase activity of calcineurin against physiological substrates. FKBP12/FK506 does not, however, bind at the phosphatase active site.

35 Thus, a compound may inhibit calcineurin by binding to the phosphatase active site ("active site"), by binding to an accessory binding site, such as the

- 3 -

FKBP12/FK506 binding site, or by binding to both sites simultaneously. Such compounds may interact directly with calcineurin or, alternatively, may bind to FKBP12, or a FKBP12 homologue, prior to binding to calcineurin.

5

FKBP12 has been characterized by its cDNA and amino acid sequences. The crystal structures of FKBP12, and of FKBP12 bound to FK506, have been reported. However, this structural information has not proven useful in the design of calcineurin inhibitors [M. V. Caffrey et al., Bioorg. Med. Chem. Lett., 21, pp. 2507-2510 (1994)].

10

Rat calcineurin has been characterized by its amino acid sequences and its cDNA. Human calcineurin has been characterized by its amino acid sequences and its cDNA [Guerini et al., Proc. Natl. Acad. Sci. USA, 86, pp. 9183-87 (1989)]. Knowledge of the primary structure, i.e., amino acid sequence, of calcineurin, however, does not allow prediction of its tertiary structure. Nor does it afford an understanding of the structural, conformational, and chemical interactions of calcineurin with FKBP12/FK506 or other compounds or inhibitors.

15

20

The crystal structure of calcineurin has not been reported. Nor has the crystal structure of a calcineurin homologue or a calcineurin co-complex been reported. The need, therefore, exists for determining the crystal structure of calcineurin to provide a more accurate description of the structure of calcineurin to aid in the design of improved inhibitors of calcineurin activity. The crystal structure of a complex comprising calcineurin A, calcineurin B, FKBP12, and FK506 would provide such a description.

25

30

Calcineurin inhibitors, such as FK506, have therapeutic potential as immunosuppressants. Specifically, such compounds may be used in the treatment of transplant rejection and autoimmune diseases, such as rheumatoid arthritis, multiple sclerosis, juvenile

diabetes, asthma, inflammatory bowel disease, and other autoimmune diseases.

#### SUMMARY OF THE INVENTION

Applicants have solved this problem by achieving, for the first time, the crystallization and three-dimensional structure determination of a calcineurin/FKBP12/FK506 complex and have solved the three-dimensional structure of that complex. This has allowed applicants to determine the key structural features of calcineurin, particularly the shape of its FKBP12/FK506 binding pocket and its phosphatase active site binding pocket.

Thus, the present invention provides molecules or molecular complexes that comprise either one or both of these binding pockets or homologues of either binding pocket that have similar three-dimensional shapes.

The invention also provides machine readable storage medium which comprises the structural coordinates of either one or both of these calcineurin binding pockets, or similarly shaped, homologous binding pockets. Such storage medium encoded with these data are capable of displaying a three-dimensional graphical representation of a molecule or molecular complex which comprises such binding pockets on a computer screen or similar viewing device.

The invention also provides methods for designing, evaluating and identifying compounds which bind to the aforementioned binding pockets. Such compounds are potential inhibitors of calcineurin or its homologues.

The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to calcineurin. This is achieved by using at least some of

the structural information obtained for the calcineurin complex.

5           The invention also provides a method for crystallizing a calcineurin/FKBP12/FK506 complex and related complexes by removing the C-terminal portion of calcineurin subunit A.

#### BRIEF DESCRIPTION OF THE FIGURES

10           Figure 1 lists the atomic structure coordinates for a bovine brain CnA/CnB/FKBP12/FK506 complex as derived by X-ray diffraction from a crystal of that complex. The following abbreviations are used in Figure 1:

15           "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

20           "X, Y, Z" crystallographically define the atomic position of the element measured.

25           "B" is a thermal factor that measures movement of the atom around its atomic center.

30           "Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

35           Figure 2 depicts the structure of the calcineurin A, calcineurin B, FKBP12, and FK506 co-complex as determined from x-ray crystallography.

40           Figure 3 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 4 and 5.

45           Figure 4 shows a cross section of a magnetic storage medium.

50           Figure 5 shows a cross section of a optically-readable data storage medium.

DETAILED DESCRIPTION OF THE INVENTION

The following abbreviations are used throughout the application:

A = Ala = Alanine	T = Thr = Threonine
V = Val = Valine	C = Cys = Cysteine
L = Leu = Leucine	Y = Tyr = Tyrosine
I = Ile = Isoleucine	N = Asn = Asparagine
P = Pro = Proline	Q = Gln = Glutamine
F = Phe = Phenylalanine	D = Asp = Aspartic Acid
W = Trp = Tryptophan	E = Glu = Glutamic Acid
M = Met = Methionine	K = Lys = Lysine
G = Gly = Glycine	R = Arg = Arginine
S = Ser = Serine	H = His = Histidine

15           CnA = calcineurin subunit A  
CnB = calcineurin subunit B

Additional definitions are set forth in the specification where necessary.

20           In order that the invention described herein may be more fully understood, the following detailed description is set forth.

25           Applicants have solved the three-dimensional structure of a calcineurin/FKBP12/FK506 complex using high resolution X-ray crystallography. Importantly, this has provided, for the first time, the information about the shape and structure of both the calcineurin active site binding pocket and the auxiliary FKBP12/FK506 binding pocket.

30           Binding pockets are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association

with the binding pockets of receptors and enzymes. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is crucial in designing potential inhibitors of calcineurin-like binding pockets.

The term "binding pocket", as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound.

The term "calcineurin-like binding pocket" refers to a portion of a molecule whose shape is sufficiently similar to either the active site binding pocket or FKBP12/FK506 binding pocket as to bind common ligands. This commonality of shape is defined by a root mean square deviation from the structure coordinates of the backbone atoms of the amino acids that make up that binding pocket in calcineurin (as set forth in Figure 1) of not more than 1.5Å. How this calculation is obtained is described below.

The "active site binding pocket" or "active site" of calcineurin refers to the site where dephosphorylation of a substrate occurs. In resolving the crystal structure of bovine brain calcineurin applicants have determined that calcineurin subunit A amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 are situated close enough to a phosphate molecule present in the active site (within 8 Å) to interact with it. It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of calcineurin may be different than that isolated from bovine brain.

Each of those amino acids is defined by a set of structure coordinates as set forth in Figure 1. The term "structure coordinates" refers to Cartesian

coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a calcineurin complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations caused by acceptable errors in the individual coordinates will have little, if any effect on overall shape. In terms of binding pockets, these acceptable variations would not be expected to alter the nature of ligands that could associate with those pockets.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a calcineurin molecule or portions thereof. The association may be non-covalent -- wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

The variations discussed above may be generated because of mathematical manipulations of the CnA/CnB/FK506/FKBP12 structure coordinates. For example, the structure coordinates set forth in Figure 1 could be manipulated by crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of

the raw structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions and deletions of amino acids in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same. Thus, for example, a ligand that bound to the active site binding pocket of calcineurin would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the acceptable error. Such modified complexes or the binding pocket(s) thereof are also within the scope of this invention.

A third possible variant is an unrelated molecule or molecular complex which contains a binding pocket that has a similar shape as a calcineurin binding pocket. The binding pocket of that unrelated molecule would also be expected to bind ligands that are capable of binding to the calcineurin binding pocket.

Various computational analyses are therefore necessary to determine whether a molecule or the binding pocket portion thereof is sufficiently similar to either of the two calcineurin binding pockets described above. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., Waltham, MA) version 3.3, and as described in the accompanying User's Guide, Volume 3 pgs. 134-135.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define

the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA is defined by user input, for the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, C $\alpha$ , C and O) for all conserved residues between the two structures being compared. We will also consider only rigid fitting operations.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses a least squares fitting algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any set of structure coordinates of a molecule or molecular complex or a binding pocket thereof that has a root mean square deviation of conserved residue backbone atoms (N, C $\alpha$ , C, O) of less than 1.5 $\text{\AA}$  when superimposed -- using backbone atoms -- on the relevant structure coordinates listed in Figure 1 are considered identical. More preferably, the root mean square deviation is less than 1.0 $\text{\AA}$ . Most preferably, the root mean square deviation is less than 0.5 $\text{\AA}$ .

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a

protein from the backbone of calcineurin or a binding pocket portion thereof, as defined by the structure coordinates of calcineurin described herein.

5       The term "least squares" refers to a method based on the principle that the best estimate of a value is that in which the sum of the squares of the deviations of observed values is a minimum.

10      Therefore, according to one embodiment, the present invention provides a crystallized molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex comprising a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

15      Preferably, the crystallized molecule or molecular complex comprises a binding pocket that is defined by structure coordinates of those CnA amino acids that are situated within 5Å of the phosphate molecule in the crystal, i.e., amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 281, 282, 283, 306, 311, 199, 232, and 254 according to Figure 1, or a binding pocket, wherein that has a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å.

20      Applicants' elucidation of the calcineurin/FKBP12/FK506 crystal structure has also revealed the details about the FKBP12/FK506 binding pocket. An FKBP12/FK506 complex is capable of binding to calcineurin at a site separate from the active site. Because the binding of that complex inhibits calcineurin-mediated activities, the elucidation of the binding site provides a second area on which new inhibitors may be modelled. The crystal structure revealed a subset of

calcineurin amino acids that were close enough to interact with the bound FKBP12/FK506 complex.

Therefore, according to an alternate embodiment, the invention provides a crystallized molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363, and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 amino acids according to Figure 1, or a homologue of said molecule or molecular complex comprising a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

According to a more preferred embodiment, the molecule or molecular complex comprises two binding pockets. One is defined by the structure coordinates of the amino acids that make up the calcineurin active site binding pocket ± a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å. The other is defined by the structure coordinates of the amino acids that make up the calcineurin FKBP12/FK506 binding pocket ± a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å.

Even more preferred are molecules or molecular complexes that are defined by the entire set of structure coordinates in Figure 1 ± a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å. An alternative more preferred embodiment of this invention is a molecular complex that comprises amino acids 17-392 of CnA, amino acids 5-169 of CnB, FKBP12 and FK506.

In order to use the structure coordinates generated for the CnA/CnB/FKBP12/FK506 complex or one of its binding pockets or homologues thereof, it is necessary to convert them into a three-dimensional shape.

This is achieved through the use of commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

5 Therefore, according to another embodiment of this invention is provided a machine-readable storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is  
10 capable of displaying a graphical three-dimensional representation of any of the molecule or molecular complexes of this invention that have been described above.

15 According to one embodiment, the machine-readable storage medium is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253,  
20 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than  
25 1.5Å. More preferably, the binding pocket is defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232 and 254, according to Figure 1 ± a root mean square deviation from the backbone atoms of said  
30 amino acids of not more than 1.5Å.

According to another embodiment, the machine-readable storage medium is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and

CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

More preferably, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex that comprises two binding pockets. One binding pocket is defined by the structure coordinates of the amino acids that make up the calcineurin active site binding pocket ± a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å. The other is defined by the structure coordinates of the amino acids that make up the calcineurin FKBP12/FK506 binding pocket ± a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å.

Even more preferred is a machine-readable data storage medium that is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex that is defined by the structure coordinates of all of the amino acids in Figure 1 ± a root mean square deviation from the backbone atoms of those amino acids of not more than 1.5Å.

According to an alternate embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of the structural coordinates set forth in Figure 1, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

Figure 3 demonstrates one version of these embodiments. System 10 includes a computer 11 comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bidirectional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the

hardware system 10 are included as appropriate throughout the following description of the data storage medium.

Figure 4 shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of Figure 3. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24.

The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of Figure 3.

Figure 5 shows a cross section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system 10 of Figure 3. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium 100 preferably has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective

coating 114, which preferably is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112.

5                  The arrangement of the domains encodes the data as described above.

10                Thus, in accordance with the present invention, data capable of displaying the three dimensional structure of calcineurin and portions thereof and their structurally similar homologues is stored in a machine-readable storage medium, which is capable of displaying a graphical three-dimensional representation of the structure. Such data may be used for a variety of purposes, such as drug discovery.

15                For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. This provides insight into calcineurin's ability to associate with the chemical entities. Chemical entities that are capable of 20                associating with calcineurin may inhibit calcineurin. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection 25                of the structure's association with chemical entities.

30                Thus, according to another embodiment, the invention provides a method for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of: a) employing computational means 35                to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular

complex; and b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities, including inhibitory compounds, capable of binding to calcineurin-like binding pockets. Such chemical entities may interact directly with such pockets, in areas adjacent to those pockets or, alternatively, may interact with FKBP12, or a homologue or mutant of FKBP12, and the resulting complex may interact with the binding pocket. Such chemical entities and compounds, optionally bound to FKBP12, may interact with either or both calcineurin-like binding pockets, in whole or in part. Preferably, if the entity binds to FKBP12, the resulting complex interacts with the calcineurin-like binding pocket that corresponds to the FKBP12/FK506 binding site on calcineurin.

Portions of both FKBP12 and FK506 participate in the binding of that complex to the FKBP12/FK506 binding site of calcineurin. Therefore, inhibitors that bind to a corresponding calcineurin-like binding site may be designed to mimic the interactions of that entire complex with the binding site. Alternatively, if the inhibitor is capable of complexing with FKBP12, it need only mimic the interactions of the FK506 portion of the FKBP12/FK506 complex with the binding site.

The crystal structure of the FKBP12/FK506 complex has been solved and has aided in the design of new compounds that bind to FKBP12 [D. A. Holt et al., J. Am. Chem. Soc., 115, pp. 9925-38 (1993)]. However, none of those compounds when bound to FKBP12 have been satisfactory in inhibiting calcineurin [M. V. Caffrey et al., Bioorg. Med. Chem. Letts., 4, pp. 2507-10 (1994)].

Accordingly, applicants' elucidation of the FKBP12/FK506 binding site on calcineurin provides the necessary information for designing compounds that when bound to FKBP12 are able to bind to the corresponding calcineurin-like binding site.

Throughout this section, discussions about the ability of an entity to bind to, associate with or inhibit a calcineurin-like binding pocket refers to features of the entity alone, or as part of a complex with FKBP12 or naturally occurring FKBP12 isoforms and homologues. Assays to determine if a compound binds to FKBP12 are well known in the art [M. W. Harding et al., Nature, 341, pp. 758-60 (1989); J. J. Siekierka et al., Nature, 341, pp. 755-57 (1989)].

The design of compounds that bind to or inhibit calcineurin-like binding pockets according to this invention generally involves consideration of two factors. First, the entity must be capable of physically and structurally associating with the calcineurin-like binding pocket. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

Second, the entity must be able to assume a conformation that allows it to associate with the calcineurin-like binding pocket directly. Although certain portions of the entity will not directly participate in these associations, those portions of the entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several chemical entities that directly interact with the

calcineurin-like binding pocket or FKBP12 or homologues thereof.

5       The potential inhibitory or binding effect of a chemical entity on a calcineurin-like binding pocket may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the calcineurin-like binding pocket testing of the entity is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to a calcineurin-like binding pocket. This may be achieved by testing the ability of the molecule to inhibit calcineurin using the 10 assays described in Examples 6 and 7. In this manner, synthesis of inoperative compounds may be avoided.

15

20       A potential inhibitor of a calcineurin-like binding pocket may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the calcineurin-like binding pockets.

25       One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a calcineurin-like binding pocket. This process may begin by visual inspection of, for example, a calcineurin-like binding pocket on the computer screen based on the calcineurin coordinates in Figure 1 or other coordinates which define 30 a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined supra. Docking may be accomplished using software such as Quanta 35 and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

- 5 1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.
- 10 2. MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, MA.
- 15 3. AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.
- 20 4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of calcineurin. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

- 35 1. CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems, Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, CA.
- 40 2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in

Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992).

3. HOOK (available from Molecular Simulations, Burlington, MA).

5 Instead of proceeding to build an inhibitor of a calcineurin-like binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other calcineurin binding compounds may be designed as a whole or "de novo" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). These methods include:

- 15 1. LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, CA.
- 20 2. LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, MA.
3. LeapFrog (available from Tripos Associates, St. Louis, MO).

25 Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

30 Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to a calcineurin-like binding pocket may be tested and optimized by computational evaluation. For example, an effective calcineurin-like binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient calcineurin-like binding pocket inhibitors

should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. Calcineurin-like binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to a calcineurin-like binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the protein when the inhibitor is bound to FKBP12 or a calcineurin-like binding pocket, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1992]; AMBER, version 4.0 [P.A. Kollman, University of California at San Francisco, ©1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, MA ©1994]; and Insight II/Discover (Biosyrm Technologies Inc., San Diego, CA ©1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS 4D/35 or IBM RISC/6000 workstation model 550. Other hardware systems and software packages will be known to those skilled in the art.

Once the calcineurin binding-pocket inhibitory entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to a calcineurin-like binding pocket by the same computer methods described in detail, above.

Another approach made possible and enabled by this invention, is the computational screening of small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to a calcineurin-like binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. E. C. Meng et al., J. Comp. Chem., 13, pp. 505-524 (1992).

The structure coordinates set forth in Figure 1 can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex comprising the steps of:

- crystallizing said molecule or molecular complex;
- generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and
- applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray

diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex.

5 By using molecular replacement, all or part of the structure coordinates of the CnA/CnB/FKBP12/FK506 complex as provided by this invention (and set forth in Figure 1) can provide an accurate structure determination for all or part of an unknown crystallized molecule or molecular complex more quickly and efficiently than attempting to determine such information ab initio.

10 Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly.

15 Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide 20 an accurate estimate of the phases for the unknown structure.

25 Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the CnA/CnB/FKBP12/FK506 complex according to Figure 1 within the unit cell of the unknown molecule or molecular complex so as best to account for the observed X-ray 30 diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to give an approximate Fourier synthesis of the structure whose 35 coordinates are unknown. This, in turn, can be subjected to any well-known refinement technique to provide a final, accurate structure of the unknown crystal. E.

Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972).

5           The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to a portion of the CnA/CnB/FKBP12/FK506 can be resolved by this method.

10          In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about a molecule or molecular complex, wherein the complex comprises at least one catalytically functional calcineurin A subunit. The term "catalytically functional calcineurin A subunit refers" to calcineurin A, as well as fragments and structural homologues thereof which retain their phosphatase activity.

20          The structure coordinates of calcineurin as provided by this invention are particularly useful in solving the structure of other crystal forms of the CnA/CnB/FKBP12/FK506 complex.

25          Furthermore, the structure coordinates of calcineurin as provided by this invention are useful in solving the structure of calcineurin mutants, which may optionally be crystallized in co-complex with a chemical entity. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type calcineurin. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between calcineurin and a chemical entity or compound.

35          The structure coordinates are also particularly useful to solve the structure of crystals of calcineurin or calcineurin homologues co-complexed with a variety of

chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate calcineurin inhibitors and calcineurin. For example, 5 high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their calcineurin 10 inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3Å resolution X-ray data to an R value of about 0.20 or less using computer software, such 15 as X-PLOR (Yale University, ©1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985). This information may thus be used to optimize known 20 calcineurin inhibitors, and more importantly, to design and synthesize new calcineurin inhibitors.

In another embodiment of this invention is provided a method for preparing a CnA/CnB/FKBP12/FK506 crystal comprising the steps of forming a molecular complex between FKBP12, FK506, calcineurin A and calcineurin B; digesting the molecular complex with a protease that removes the calmodulin binding site and the autoinhibitory domain of calcineurin A; and crystallizing the digested complex. 25

In another embodiment of this invention is provided a method for preparing a CnA/CnB/FKBP12/FK506 crystal comprising the steps of forming a molecular complex between FKBP12, FK506, calcineurin A and calcineurin B; wherein calcineurin A lacks a calmodulin 30 binding domain and an autoinhibitory domain; and crystallizing the complex.

- 28 -

The autoinhibitory domain of CnA has been mapped to the C-terminal 4 kDa of that polypeptide. The calmodulin binding domain is located adjacent to the autoinhibitory domain and occupies up to 14kDa. Thus, an N-terminal 43 kDa fragment of CnA lacks both domains [M. J. Hubbard et al., Biochemistry, 28, pp. 1868-74 (1989)]. Removal of the calmodulin binding domain and the autoinhibitory domain does not appear to affect the active site or FKBP12/FK506 binding sites, nor the ability of CnA to bind to CnB. Removal of the calmodulin binding site and the autoinhibitory site does, however, provide a complex that provides stable crystals, suitable for analysis by X-ray crystallography.

The removal of the autoinhibitory and calmodulin domains may be carried out either before or after calcineurin is bound to the FKBP12/FK506 complex. Removal of these domains is preferably achieved by proteolytic digestion or through recombinant DNA techniques.

Preferably, the protease is selected from the group consisting of clostripain, trypsin, endoproteinase Lys-C, endoproteinase Asp-N, endoproteinase Glu-C, elastase, enterokinase, restriction protease Factor Xa, thermolysin (Altus Biologics, Cambridge, MA), II-1 beta converting enzyme or HIV-1 protease. Most preferably, the protease is clostripain.

Preferably, the processed CnA subunit in the crystallized complex has a molecular weight of about 42kDa.

In order that the invention described herein may be more fully understood, the following examples are set forth. It should be understood that these examples are for illustrative purposes only and are not to be construed as limiting this invention in any manner.

EXAMPLE 1Purification of Calcineurin A/Calcineurin B

Bovine calcineurin was isolated from calf brains (1 year old, or less), essentially as described by Sharma and Wang. (R. K. Sharma et al., J. Biol. Chem. 261, pp. 1322-1328 (1986)). This procedure yields a mixed population of calcineurin isozymes and a small proportion of non-calcineurin contaminants. Most of the non-calcineurin contaminants were removed by anion exchange chromatography. The crude calcineurin fraction was exchanged into buffer A (20 mM Tris-HCl, 2 mM  $\beta$ -mercaptoethanol, 1 mM magnesium acetate, 1 mM imidazole, 0.1 mM EGTA, 0.1 mM PMSF, pH 7.6 at 4°C), by dialysis or ultrafiltration, at a protein concentration of 0.5 - 2 mg/ml. The protein was loaded onto a column (2.5 x 20 - 30 cm) of DEAE-Sephadex (Pharmacia) that had been pre-equilibrated, at 4°C, in the same buffer. After loading the protein, the column was washed with 2 - 5 column volumes of buffer A, and then the bound proteins were eluted from the column with a linear gradient of 0-300 mM NaCl (10 column volumes), in the same buffer system, at 4°C. The calcineurin, eluting as the main peak, was then fractionated into numerous isoforms by hydrophobic interaction chromatography. The protein was exchanged into buffer B (50 mM Tris-HCl, 1.4 M ammonium sulfate, 5% (v/v) glycerol, 2 mM  $\beta$ -mercaptoethanol, 1 mM EGTA, pH 7.5 at 20°C), and loaded onto a Hydopore-HIC (Rainin) column (2.0 x 30 cm) pre-equilibrated in the same buffer. The calcineurin isozymes were eluted at 20°C with a linear gradient (8 column volumes) from 1.4 M to 0 M ammonium sulfate, keeping the other buffer components constant. The first peak representing about 60% of the total was designated as the "major isoform." The A and B subunits were of this major isoform were separated by reversed phase HPLC and SDS PAGE. Peptide mapping of the fractionated subunits, followed by amino acid sequence analysis of the peptide products, generated internal

- 30 -

sequence data for both subunits. When compared with independently determined cDNA sequences (and the deduced amino acid sequences) the experimentally obtained protein sequences indicated that this major isoform consisted of intact, myristoylated calcineurin B, and intact calcineurin A. This protein was concentrated by ultrafiltration and dialyzed into buffer C (25 mM Tris-HCl, 0.1 mM MnCl<sub>2</sub>, 0.1 mM CaCl<sub>2</sub>, 2 mM β-mercaptoethanol, pH 8.0 at 4°C).

10

EXAMPLE 2

Crystallization of Calcineurin A/  
Calcineurin B/FKBP12/FK506

A binary complex of recombinant bovine FKBP12 and FK506 was prepared, essentially as described previously [K. P. Wilson et al., Acta Crystallography, in press (1995)]. This complex was exchanged into buffer C (25 mM Tris-HCl, 0.1 mM MnCl<sub>2</sub>, 0.1 mM CaCl<sub>2</sub>, 2 mM β-mercaptoethanol, pH 8.0 at 4°C), and then combined with the pure calcineurin major isoform at a molar ratio of 1:1.3 (calcineurin:FKBP/FK506 complex) and a final total protein concentration of 1-2 mg/ml. The calcineurin/FKBP12/FK506 complex was allowed to equilibrate for 1 hour at 4°C, before the addition of clostripain (IUB:4.4.22.8; Worthington) at 3 mg of clostripain per 100 mg of complex. Proteolytic digestion of the complex was allowed to proceed for 3-4 days at 4°C, before the protein was concentrated to 15-20 mg/ml (50-100 mg total protein) by ultrafiltration, and then size-fractionated at 4°C on a column system of Sephadryl S-300 HR (2.6 x 100 cm x 3) equilibrated in the same buffer (buffer C). The central 90% of the main peak, eluting soon after the void volume, was pooled. The pooled material was analyzed by SDS-polyacrylamide gel electrophoresis, reversed phase HPLC, UV absorption spectroscopy and electrospray mass spectroscopy. In addition, direct N-terminal amino acid sequence analyses

were performed on each of the polypeptide components present, and on HPLC-purified peptides from additional proteolytic mapping experiments which generated a range of internally truncated peptides. These analyses  
5 indicated that pooled material consisted, predominantly, of intact complex, containing (in approximately 1:1:1:1 stoichiometry):

- a) N- and C-terminally truncated calcineurin A (residues 17-392);
- 10 b) intact, myristoylated calcineurin B (residues 1-169);
- c) intact FKBP12; and
- d) FK506.

The added clostripain, unbound FKBP-12/FK506 complex, and  
15 the small peptide fragments (generated by clostripain-proteolysis of the calcineurin) eluted later from the size-exclusion column and were discarded.

The proteolytic processing of the complex under these conditions does not give single pure products for  
20 either the calcineurin A or the calcineurin B. The product initiation and termination points are all extremely similar, but not identical. For the A chain, cleavage at the N-terminus results in about 95%+ of the products beginning at residue 17. Approximately 5% of the products begin at residue 20. The majority of the C-terminal cleavage leaves products that appear to terminate at residue 392, since no evidence was found for other C-terminal termination points. For the calcineurin B, the majority of the products remain N-terminally  
25 blocked and, therefore, are still myristoylated, as demonstrated by the crystal structure. A small proportion (perhaps up to 25%) appears to be cleaved between residues 4 (Ala) and 5 (Ser). No evidence was found for C-terminal cleavage of the calcineurin B.  
30

35 The purified complex was concentrated by ultrafiltration to 25-55 mg/ml, and centrifuged at 40,000 x g for 10-15 minutes. Crystals were obtained from these

solutions, using hanging drops (initially 8 $\mu$ L total, 25% precipitant) suspended over a precipitant reservoir of 8% PEG 8000, 0.1 M potassium phosphate, 20 mM  $\beta$ -mercaptoethanol. Crystals appeared within 3-4 days at 5 4°C, and reached maximal size in about 2-3 weeks. SDS PAGE analysis of the redissolved crystals showed essentially identical protein composition as the original complex solution.

Those of skill in the art will appreciate that 10 the aforesaid crystallization conditions can be varied. Such variations may be used alone or in combination, and include final protein/inhibitor complex concentrations between 5 mg/ml and 35 mg/ml; all combinations of calcineurin/FKBP12/FK506 to precipitant ratios; citrate 15 concentrations between 1mM and 200 mM; DTT concentrations between 0 mM and 10 mM; and any concentration of  $\beta$ -mercaptoethanol; pH ranges between 5.5 and 9.5; PEG concentrations between 10% and 25% (g/100ml); PEG weights between 2000 and 8000; LiSO<sub>4</sub> concentrations between 50 and 20 750 mM; HEPES concentrations between 5 and 395 mM; and any concentration or type of detergent; any temperature between -5°C and 30°C; and crystallization of calcineurin/FKBP12/FK506 complexes by batch, liquid bridge, or dialysis method using these conditions or 25 variations thereof.

### EXAMPLE 3

#### Crystal Structure of Calcineurin A/ Calcineurin B/FKBP12/FK506

Initial heavy atom searches were carried out 30 with crystals stabilized in 50mM HEPES, pH 7.5, and 12% PEG 8000. Native and heavy atom derivatized crystals were transferred to 50 mM HEPES, pH 7.5, 12% PEG 8000, and 22% glycerol (w/v), and frozen at approximately -165°C in a dry nitrogen gas stream for data collection. This stabilization process changed the unit cell 35 dimensions to a=89.3 $\text{\AA}$ , b=92.1 $\text{\AA}$ , and c=118.5 $\text{\AA}$ . Two

derivatives were obtained under these conditions using di-O-iodobis(ethylenediamine)-di-platinum (II) nitrate (PIP), and Pb(NO<sub>3</sub>)<sub>2</sub>, the latter on crystals which had been treated with EGTA to remove Ca<sup>++</sup> from the metal binding sites on calcineurin B. Native and derivative data sets were collected on frozen crystals by oscillation photography on a Rigaku R-AXIS IIC phosphor imaging area detector mounted on a Rigaku RU200 rotating anode generator (Molecular Structure Corp., Houston, TX), operating at 50kV and 100mA. Measured intensities were integrated, scaled, and merged using the HKL software package (Z. Otwinowski and W. Minor, personal communication). The native data set was denoted native1 and the two derivative data sets denoted calc\_106 (PIP) and calc\_149 (Pb(NO<sub>3</sub>)<sub>2</sub>).

Heavy atom positions were located by inspection or with RSPS (Knight, S. Thesis, Swedish Univ. Agricultural Sciences (1989)) and confirmed with difference Fourier syntheses using PHASES (W. Furey et al., S. Am. Cryst. Assoc. Mtg. Summ. 18, p. 73 (1990)). Heavy atom parameters were refined with HEAVY (T. C. Terwilliger et al., Acta Crystallogr., A39, pp. 813-817 (1983)), and phases computed using either HEAVY or MLPHARE (Z. Otwinowski, ML-PHARE CCP4 Proc. 80-88 (Daresbury Laboratory, Warrington, UK, 1991)). MIR phases were improved and extended by cycles of solvent flattening (B. C. Wang, Meth. Enzym. 115, pp. 90-112 (1985)), phase combination using SIGMAA (R. J. Reed, Acta Crystallogr., A42, pp. 140-149 (1986)), and histogram matching combined with Sayre's equation (K. Y. J. Zhang et al., Acta Crystallogr., A46, pp. 377-381 (1990) using the CCP4 crystallographic package (CCP4 (1986), A Suite of Programs for Protein Crystallography, SERC Daresbury Laboratory, Warrington WA4 4WD, England)). The molecular model was built into electron density maps using QUANTA (Quanta version 4.1, Molecular Simulations Inc., Burlington MA, 1995), and the model refined with

XPLOR-3.1 (A. T. Brunger, X-PLOR (Version 3.1), Yale Univ., New Haven, (1993)).

Refinement of the PIP and Pb(NO<sub>3</sub>)<sub>2</sub> derivatives, including the anomalous contribution from the Pb(NO<sub>3</sub>)<sub>2</sub> derivative gave a figure of merit of 0.53 to 4.6Å. The resulting MIRAS map was subjected to cycles of solvent flattening, phase combination, and phase extension to produce an electron density map at 4.0Å. A partial model for calcineurin A and calcineurin B was built into this map, and FKBP12 was positioned into the density as a rigid body. The partial structure was refined against the native1 data, and then refined as a rigid body against a new native data set (denoted native2), from crystals stabilized in 0.1M potassium phosphate, pH 7.5, 12% PEG 8000, and cryoprotected with 0.1M potassium phosphate, pH 7.5, 9% PEG 8000, and 23% ethylene glycol. These conditions yielded yet another cell, with dimensions a=91.3Å, b=94.4Å, and c= 116.8. Three new derivatives soaked and cryoprotected under the same conditions as native2 were obtained with HgCl<sub>2</sub> (calc\_158), Pb(NO<sub>3</sub>)<sub>2</sub> (calc\_171), and K<sub>2</sub>PtCl<sub>6</sub> (calc\_170). Heavy atom parameter refinement for these three derivatives against native2 to 3.3Å gave a final figure of merit of 0.58, including the Pb(NO<sub>3</sub>)<sub>2</sub> anomalous data. This MIRAS map was again subjected to cycles of solvent flattening/phase extension, and multiple electron density maps were calculated ranging from 3.6 to 2.6Å resolution. The resulting maps were used to build in approximately 80% of CnA and CnB chains as polyalanine, beginning with the previous model. Multiple rounds of model building, positional refinement, phase combination, and phase extension gave improved electron density maps into which a nearly complete model was built. The positions of the lead, mercury, and platinum heavy atom sites were used to confirm the register of the sequence during building of loops and side chains in the latter stages of model building. A nearly complete model of the

CnA/CnB/FKBP12/FK506 complex was subjected to simulated annealing refinement, followed by positional and temperature factor refinement at 2.6Å. The remainder of the model along with well ordered water molecules was built into  $2|F_o - F_c|$  and  $|F_o| - |F_c|$  difference fourier maps. The current model contains residues 24-240 and 247-370 of calcineurin A, residues 5-82 and 84-168 of calcineurin B, an N-terminal myristoyl group associated with calcineurin B, residues 1-107 of FKBP12, FK506, 4 Ca<sup>++</sup> ions in the calcineurin B Ca<sup>++</sup> binding sites, 1 PO<sub>4</sub><sup>3-</sup> group, 1 Fe<sup>++</sup> ion, and 1 Zn<sup>++</sup> ion in the calcineurin A active site, and 87 waters. It has been refined using data between 6.0 and 2.5Å.

EXAMPLE 4

15        Structural Features Of The CnA/CnB/FKBP12/FK506 Crystal

The crystals had an orthorhombic space group symmetry P<sub>12121</sub>. The crystals also had a rectangular shaped unit cell, each unit cell having the dimensions a=90 ± 5Å, b=94 ± 6Å, and c=117 ± 5Å. The crystal comprised four complexes per unit cell, wherein CnA interacts with CnB, FKBP12, and FK506; CnB interacts with CnA, FKBP12, and FK506; FKBP12 interacts with CnA, CnB, and FK506; and FK506 interacts with CnA, CnB, and FKBP12.

25        The CnA subunit contained a series of amino acids within 8Å of a phosphate group and two metal ions bound to the active site. These were amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317, according to Figure 1. A subset of these, amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 281, 282, 283, 306, 311, 199, 232, and 254, were within 5Å.

30        The crystal further contained a FKBP12/FK506 binding site made up of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363 and CnB

amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162.

The components of the quaternary complex that make up the crystal associated to form a roughly rectangular structure with overall dimensions of 87x61x37 Å. CnA was the largest component of the complex and consisted mainly of a globular domain which contains the phosphatase site. This phosphatase-containing domain was characterized by a β-sandwich motif which formed the core of the enzyme. Perhaps the most striking feature of the quaternary complex was a 22 residue α-helix which extended nearly 40 Å away from the surface of the phosphatase-containing domain and contained the CnB binding helix (BBH). CnB comprised two calmodulin-like domains that, taken together, formed a hydrophobic groove which interacted with the upper surface of the calcineurin binding helix, leaving the underside completely exposed. It is to this exposed region of the BBH that the FKBP12-FK506 complex bound.

#### Architecture of calcineurin A

The CnA fragment used in this study contained only the phosphatase domain and the CnB binding region (residues 17-392). Missing from this fragment were the calmodulin binding domain and the autoinhibitory regions. The phosphatase domain formed a compact α/β sandwich while the CnB binding region consisted of a short linker followed by a single α-helix that protruded from the phosphatase domain.

#### Phosphatase domain

The phosphatase domain of CnA formed an ellipsoid with approximate dimensions 35Å x 35Å x 45Å. The core of the domain consisted of two mixed β-sheets, termed sheet 1 and sheet 2, which were flanked on one side by a mixed α/β structure and on the other side by an all α structure. The two central β-sheets formed a

distorted  $\beta$ -sandwich which contains an open and closed end. At the closed end of the  $\beta$ -sandwich sheet 2 extended above sheet 1, giving the  $\beta$ -sandwich an overall appearance similar to the greek letter  $\lambda$ . The two sheets 5 formed an angle of approximately 30°, resulting in their gradual separation from closed to open end. The inner core of the  $\beta$ -sandwich was filled almost exclusively with hydrophobic residues, with smaller side chains residing at the closed end of the core and larger, more bulky side 10 chains filling the open end. Strands  $\beta$ 6,  $\beta$ 10, and  $\beta$ 12 from sheet 1 were parallel and ran in the direction of the closed end of the sandwich, as did strands  $\beta$ 4,  $\beta$ 3,  $\beta$ 2, and  $\beta$ 14 in sheet 2. Following  $\beta$ 14, the sequence 15 formed an extended region covering approximately 24 residues before the start of the BBH. Residues 340-348, while still part of the phosphatase core, participated in multiple contacts with CnB and thus can be considered as part of the CnB binding region. Additional contacts between CnA and CnB occurred at the N-terminus of CnA and 20 in loop L1 where a salt bridge is formed between Glu-53 of CnA and Lys-134 of CnB. These interactions appeared to help stabilize the extended CnB/BBH structure.

The phosphatase active site was located above 25 the closed end of the  $\beta$ -sandwich, formed by the convergence of several loops and by a portion of sheet 2 which extends above the  $\beta$ -sandwich. Residues that formed part of the active site were located in loops L2, L3, L4, and L6 and at the C-termini of strands  $\beta$ 2 and  $\beta$ 3. The somewhat shallow active site pocket was located in the 30 middle of a larger, curved channel that runs along the top of sheet 1 and helix  $\alpha$ 9. This channel should accommodate access to the active site by larger, phosphorylated substrates and may help provide specificity through interactions with residues surrounding the phosphorylated side chain of the 35 substrate.

The active site contained two metal ion sites that are modelled as Zn<sup>2+</sup> and Fe<sup>3+</sup>, as well as a single phosphate ion, whose presence in the structure may be the result of including 100mM potassium phosphate buffer in the crystallization conditions.

The Zn<sup>2+</sup> and Fe<sup>3+</sup> atoms were separated by approximately 3.0Å in CnA and were identified in the active site on the basis of their interactions with surrounding ligands. The zinc was coordinated by the side chains Asp-118(Oδ2), Asn-150(Oδ1), His-199(Nε2) and His-281(Nδ1), and by a phosphate oxygen. The iron was coordinated by Asp-90(Oδ1), His-92(Nε2), Asp-118(Oδ2), a phosphate oxygen, and a water molecule.

The bound phosphate, in addition to coordinating both metals, was stabilized by interactions with the guanidinium groups of Arg-122 and Arg-254, and with the Nε2 of His-151. Arg-254 extended down from loop L5, which is fully 8.5Å away from the phosphate group, and was stabilized through a bidentate interaction with the carboxylate of Asp-234. His-151 was situated in the active site within hydrogen bonding distance of the most solvent exposed phosphate oxygen. Its side chain position was stabilized by a hydrogen bond to Asp-121, while the main chain conformation was stabilized by the next residue, Glu-152, which makes a pair of hydrogen bonds to main chain nitrogens surrounding the metal-bridging ligand, Asp-118.

#### Calcineurin B binding helix

The BBH was a five turn amphipathic  $\alpha$ -helix (residues 350-370) to which both CnB and the binary FKBP12-FK506 complex bound. The top half of the BBH was completely non-polar and formed a complementary surface to the hydrophobic groove formed by CnB (see below). The tip of the BBH abutted the N-terminal helix of CnB, which lay perpendicular to the axis of BBH and caps the end of

the BBH binding groove. The lower half of the BBH helix was polar except for a small hydrophobic patch near its N-terminus. This patch formed part of the contact surface with the FKBP12-FK506 complex.

5

#### Architecture of calcineurin B

The structure of CnB consisted of two globular calcium-binding domains flanked by a long C-terminal  $\beta$ -strand. Each calcium-binding domain contained two  $\text{Ca}^{2+}$ -binding EF-hand motifs. Domain 1 (residues 1 to 84) connected to domain 2 (residues 86 to 155) via an  $\alpha$ -helix that was kinked at Gly-85. Domains 1 and 2 were arranged linearly along the BBH and, together with the amphipathic C-terminal strand, forms a 33 Å long hydrophobic groove into which the top half of the BBH was embedded.

10

The three-dimensional structure of each of the pairs of EF-hands (EF1 and EF2 in domain 1, and EF3 and EF4 in domain 2) in CnB was highly conserved with those of other members of the super-family; the intra-domain calcium-calcium distances in CnB were nearly identical to those found in calmodulin, for example. In all four EF hands the  $\text{Ca}^{2+}$  ion was coordinated by five ligands. These are Asp-30, Asp-32, Ser-34, Glu-41, and the Ser-36 carbonyl oxygen for EF1, Asp-62, Asp-64, Asn-66, Glu-73, and the Gly-68 carbonyl oxygen for EF2, Asp-99, Asp-101, Asp-103, Glu-110 and the Tyr-105 carbonyl oxygen for EF3, and Asp-140, Asp-142, Asp-144, Glu-151 and the Arg-146 carbonyl oxygen for EF4.

15

The N-terminal glycine of CnB was covalently linked to myristate, a 14 carbon saturated fatty acid. The myristate group was located at the extreme end of the calcineurin complex, near the end of the BBH (Figure 2). It was connected to the N-terminal helix by a 15 residue loop, and lay against and ran parallel to the N-terminal helix of CnB, which was itself hydrophobic.

20

25

30

Structure of FKBP12-FK506

The conformation of FKBP12 in the ternary complex was nearly identical to that found in the structure of the FKBP12-FK506 binary complex (van Duyne et al., 1991a; Becker et al., 1993; Wilson et al., in press). Superposition of FKBP12 from the ternary and binary complexes gave a root-mean-square (rms) deviation of 0.59Å for C $\alpha$  atoms. Similarly, the conformations of FK506 were almost identical in the two complexes, with an rms difference of 0.21Å for all non-hydrogen atoms, excluding those from the highly flexible C21 allyl group. However, the relative position of FK506 to FKBP12 differed in the ternary and binary complexes. In the ternary complex FK506 was rotated by about 8° from the body of FKBP12, resulting in a displacement of 1.7Å for the C21 carbon at the base of the allyl group. A concomitant displacement of the His-87 to Ile-90 loop in FKBP12 was observed as well. This rotation allowed the allyl, and to a lesser extent, cyclohexyl moieties of FK506 to more intimately contact the BBH. One consequence of this rotation was the loss of a hydrogen bond between the Glu-54 carbonyl oxygen of FKBP12 and the C24 hydroxyl group of FK506 in the ternary complex.

FKBP12-FK506 binding to calcineurin

The FKBP12-FK506 complex bound to calcineurin at the base of the BBH making contacts with the BBH, CnB, and the phosphatase domain of CnA. The solvent accessible surface area lost to each component upon FKBP12-FK506 binding was 320Å<sup>2</sup>, 479Å<sup>2</sup>, and 512Å<sup>2</sup>. The FKBP12-calcineurin contacts surrounded the FK506 ligand and clustered to three distinct regions of the FKBP12 sequence: His-87 to Ile-90, Asp-37 to Asp-41, and Arg-42 to Phe-46. These regions contacted the BBH, the phosphatase domain, and CnB, respectively.

The principal site of interaction between FK506 and calcineurin was a predominantly hydrophobic cleft

located at the interface of CnB and the BBH. Side chains  
that formed the cleft came from residues Leu-343,  
Pro-344, Trp-352, Ser-353 (C $\beta$ ), and Phe-356 on the BBH  
and residues Leu-115, Met-118, Val-119 and Leu-123 from  
5 CnB. This binding cleft was approximately 8 Å long, and  
had surface properties complementary to the C15-C21  
region of FK506. The majority of contacts made by FK506  
were from C15 through C17 and the C21 allyl group. The  
allyl group extended into a deep pocket within the  
10 hydrophobic cleft, making a number of favorable  
van der Waals contacts with main chain and side chain  
atoms. The FK506-calcineurin interaction was further  
stabilized by an unusual bifurcated hydrogen bond between  
15 Nε1 of Trp-352 and the C13 and C15 methoxy oxygens of  
FK506.

Figure 2 depicts the structure of the calcineurin A, calcineurin B, FKBP12, and FK506 subunits as determined by x-ray crystallography.

#### EXAMPLE 5

##### Use of Calcineurin A/Calcineurin B/FKBP12/FK506

20 The coordinates in Figure 1 are used to design compounds, including inhibitory compounds, that associate with calcineurin or homologues of calcineurin, directly or through prior complexation with FKBP12 or a FKBP12 homologue. This process may be aided by using a machine-readable data storage medium encoded with a set of machine-executable instructions, wherein the recorded instructions are capable of displaying a three-dimensional representation of the CnA/CnB/FKBP12/FK506 complex or a portion thereof. The graphical representation is used according to the methods described herein to design compounds, including an inhibitory compound, that bind to calcineurin. Such compounds may associate with calcineurin at the active site, the

FKBP12/FK506 binding site, or both sites or at adjacent area to either or both of these sites.

FKBP12/FK506 binding site inhibitors

The process outlined above is used to design a compound that inhibit calcineurin by associating with the FKBP12/FK506 binding site. Such a compound binds first to FKBP12 or a variant of FKBP12 and then associates with the FKBP12/FK506 binding site. This compound consists of a hydrophobic moiety capable of making van der Waal's contact with one or more of the following residues on FKBP12: Trp59, Phe46, Tyr26, Val55, Phe99, and Ile56. Substituted onto this hydrophobic core is a hydrogen bond acceptor capable of forming a hydrogen bond with Ile56 on FKBP12 and a second hydrogen bond acceptor or a hydrogen bond donor that can form a hydrogen bond with Tyr82 on FKBP12. The binding core also contains a linker that projects a hydrophobic moiety 10-14 Å from the center of the binding core to make van der Waal's contact with one or more of the following residues: Leu115, Val119, Met118 of CnB and Trp352, Ser353, Phe356 and Val357 on CnA. The binding core also contains a second linker that projects a moiety 7-11 Å from the center of the binding core to make van der Waal's contact with one or more of the following residues: Leu123 on CnB and Leu343, Tyr341, Pro344 and Trp352 on CnA and may optionally act as a hydrogen bond acceptor with Trp352 and/or a hydrogen bond donor or acceptor with Tyr341. The binding core contains a third linker that projects a moiety 8-12 Å from the center of the binding core to make van der Waal's contact with one or more of the following residues: Pro355 and Phe356 and may optionally act as a hydrogen bond donor with Glu359 on CnA. This third linker will also make van der Waal contact with Tyr82, Ile56 and His87 on FKBP12. This molecule contains fewer than three secondary amide bonds and has a molecular weight of less than 1000.

Active site inhibitors

In another example, the process outlined above is used to design compounds that inhibit calcineurin by associating directly with the phosphatase active site. Such compounds will contain either a phosphate residue or a surrogate for a phosphate residue and additional functionality that imparts affinity for calcineurin.

The process outlined above could also be used to design compounds that inhibit calcineurin by blocking access to the active site. Examples of clefts in the enzyme that may be blocked are described by the following groups of CnA amino acids, as set forth in Figure 1:

a) Arg122, Phe125, Asp313, His339, Pro340, Tyr341, Trp342, Phe346, Tyr124, Thr161, Pro344, Phe160 and Asn345;

b) Trp232, Leu231, Pro221, His155, Glu220, Leu156, Cys153, Asn150, Pro222, Cys256, Gly255 and Arg148; and

c) Leu302, Pro235, Glu282, Phe239, Tyr291, Gln284, Thr304, Phe259, Leu236, Glu237, Val253, Ala283 and Asp234.

Compounds that make contact primarily with any of these three sets of residues would be active site inhibitors.

EXAMPLE 6Calcineurin Inhibition Assay

The calcineurin assay is performed essentially as described by Klee and Cohen [C. V. Klee et al., Mol. Aspects Cell. Regul., 5, pp. 225-248 (1988)].

A commercial preparation of bovine brain calcineurin is used (Sigma, Cat# C-1907, specific activity = 16 nmol/min/mg under the conditions of the assay). Radiolabeled phosphorylated peptide substrate, derived from the serine phosphorylation site sequence of the RII subunit of cAMP-dependent protein kinase, is prepared as described previously [R. A. Aldape et al., J. Biol. Chem. 267, pp. 16029-16032 (1992)].

The serine phosphatase assay is performed in 60 $\mu$ l buffer containing 20 mM Tris, pH 8.0, 0.1M NaCl, 6mM MgCl<sub>2</sub>, 0.1 mM CaCl<sub>2</sub>, 0.5 mM dithiothreitol, and 0.1 mg/ml bovine serum albumin (C. V. Klee et al, supra). The following ordered additions are made for the assays: 5nM - 15 $\mu$ M FKBP, 5nM - 15 $\mu$ M FK506, 160 nM bovine calmodulin (Sigma, Cat# P-277) and 40 nM bovine brain calcineurin. [<sup>32</sup>P]-phosphorylated peptide is added to 1-2 $\mu$ M final concentration, followed by a 15 min incubation at 30°C.

Reactions are quenched with 540  $\mu$ l 0.1M potassium phosphate/5% trichloracetic acid (w/v). Cation exchange columns (Dowex AG1-X8, 0.6 ml) are used for separation of free [<sup>32</sup>P]-P<sub>i</sub> (M. J. Hubbard et al., in Molecular Neurobiology: A Practical Approach, J. Chad et al., Eds. (Oxford University Press, Oxford, England) pp. 135-149, 1991). The quenched reaction mixtures (0.6 ml) are applied to the columns, followed by a 0.6 ml H<sub>2</sub>O wash, and the effluents are collected in scintillation vials and counted with 5 ml of scintillation cocktail (Beckmann Liquiscint). All assays are performed in duplicate.

Affinity of the FKBP-test ligand complexes for calcineurin is determined by varying the concentrations of FKBP and test ligand at 30°C, using a drug:FKBP ratio of 1.35:1. FK506:test ligand ratios are increased appropriately for the lower affinity ligands to ensure saturation of the FKBP with test ligand.

#### Data Analysis

The inhibition constant for calcineurin by the FKBP/test ligand complexes (K<sub>ic</sub>) is calculated by computer-fitting the fractional inhibition data as a function of concentration of free FKBP and test ligand to an the equilibrium equation derived by Liu et al [J. Liu, et al., Biochemistry, 31, pp. 3896-3901 (1992)]. Quadratic equations are first used to calculate the free concentrations of these reaction components from the concentrations of calcineurin, FKBP and test ligand in

- 45 -

the experiment, as well as the  $K_i$  of the FKBP for test ligand. The calcineurin affinity of the FKBP/test ligand complex is calculated using the equation:  $I/(1-I) = [TestLigand]_{free}[FKBP12]_{free}/(K_i K_{ic})$ , where I is the fractional inhibition of calcineurin and (1-I) is the fractional activity remaining.  $K_{ic}$  and the associated standard deviation are calculated from the linear regressions performed on MiniTab (Addison-Wesley).

EXAMPLE 7

10                   Immunosuppression (Mitogenesis)  
                      Assays Cell Source and Culture

Fresh peripheral blood lymphocytes (PBLs) from LeukoPak cells or whole blood from random normal blood donors (tested HIV-negative and hepatitis negative) are isolated and separated by density centrifugation over Histopaque 1077 (Sigma Chemical Co., St. Louis, MO). The murine CTLL cytotoxic T cell line and the human Jurkat T cell line are available from ATCC (CTLL-2 ATCC TIB214, JURKAT CLONE E6-1 ATCC TIB152). The human allogeneic B cell lines used for activation of the fresh PBLs are EBV-transformed lymphocytes from normal healthy adult donors with two completely different HLA haplotypes. All cell lines are routinely tested for the presence of Mycoplasma contamination using the Gibco Mycotect test kit and found to be Mycoplasma-free. Culture medium consisted of RPMI 1640 (Gibco, Grand Island, NY) containing penicillin (50 U/ml) and streptomycin (50 µg/ml), L-glutamine 2 mM, 2 mercaptoethanol ( $5 \times 10^{-5}$ ), 10% heat-inactivated FCS and 10 mM HEPES.

30                   Compound Solutions and Titrations

All chemical stocks are dissolved in DMSO. Titrations of compounds are made into the medium the individual assay are carried out in, i.e., complete RPMI or HB 104 for final diluted concentrations, using

multiple three-fold dilutions from 1  $\mu\text{M}$  or 10  $\mu\text{M}$  stock solutions.

Mitogenesis Assays ("PMA" and "OKT3")

The inhibitory effect of test compounds on the proliferation of human PBLs in response to mitogens (W. K. Waithe et al., Handbook of Experimental Immunology, 3d Ed., Blackwell Scientific Publications, Oxford (1978); B.B. Mishell et al., Selected Methods in Cellular Immunology, W. H. Freeman and Co., San Francisco, CA (1980)) are assessed by stimulation of  $5 \times 10^4$  cells with OKT3 ( $10^{-4}$  dilution final) or PMA (10 ng/ml) plus ionomycin (250 ng/ml) in the presence or absence of different concentrations of test compounds and control drugs (CsA, FK506, rapamycin) in final volume of 200  $\mu\text{l}$  per well in 96 well round bottomed plates. After 48 h incubation ( $37^\circ\text{C}$ , 5%  $\text{CO}_2$ ), cells are pulsed with 1  $\mu\text{Ci}$  of  $^3\text{H}$ -Leucine, harvested 24 h later with a Tom Tek cell harvester, and counted in LKB  $\beta$ -scintillation counter. Results (cpm) are compared with controls with medium alone, and concentrations causing 50% reduction in counts ( $\text{IC}_{50}$ ) are calculated.

While we have described a number of embodiments of this invention, it is apparent that our basic examples may be altered to provide other embodiments which utilize the products and processes of this invention. Therefore, it will be appreciated that the scope of this invention is to be defined by the appended claims rather than by the specific embodiments which have been represented by way of example.

CLAIMS

We claim:

1. A crystallized molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

2. The crystallized molecule or molecular complex according to claim 1, wherein said binding pocket is defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

3. A crystallized molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 123, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

4. The crystallized molecule or molecular complex according to claim 1, further comprising a second

- 48 -

binding pocket defined by CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162; according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a second binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

5. The crystallized molecule or molecular complex according to claim 4, wherein said molecule or molecular complex is defined by the set of structure coordinates according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

6. The crystallized molecule or molecular complex according to claim 4, wherein said molecule or molecular complex comprises amino acids 17-392 of CnA, CnB, FKBP12 and FK506.

7. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- 49 -

8. The machine-readable storage medium according to claim 7, wherein said binding pocket is defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

9. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

10. The machine-readable data storage medium according to claim 7, wherein said molecule or molecular complex further comprises a second binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a second binding pocket

that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

11. The machine-readable data storage medium according to claim 10, wherein said molecule or molecular complex is defined by the set of structure coordinates according to Figure 1, or a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

12. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates according to Figure 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

13. A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex according to any one of claims 1 to 6 comprising the steps of:

- a. employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and
- b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

- 51 -

14. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex comprising the steps of:

a. crystallizing said molecule or molecular complex;

b. generating an X-ray diffraction pattern from said crystallized molecule or molecular complex;

c. applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction pattern to generate a three-dimensional structure of at least a portion of the molecule or molecular complex.

15. The method according to claim 14, wherein the molecule or molecular complex comprises a polypeptide selected from a catalytically functional calcineurin A subunit.

16. A method for preparing a CnA/CnB/FKBP12/FK506 crystal comprising the steps of:

a. forming a molecular complex between FKBP12, FK506, calcineurin A and calcineurin B, wherein the calcineurin A lacks a calmodulin binding domain and an autoinhibitory domain; and

b. crystallizing the digested complex.

17. The method according to claim 16, wherein the calmodulin binding domain and the autoinhibitory domain of said calcineurin A are removed by proteolytic digestion with a protease selected from clostripain, trypsin, endoproteinase Lys-C, endoproteinase Asp-N, endoproteinase Glu-C, elastase, enterokinase, restriction protease Factor Xa, thermolysin, IL-1 beta converting enzyme or HIV-1 protease

18. The method according to claim 17, wherein the protease is clostripain and the calcineurin A subunit in

- 52 -

the crystallized complex has a molecular weight of about 42 kDa.

1/145

FIGURE 1FKBP12 COORDINATES

		Atom	Type	Residue #	X	Y	Z	OCC	B
ATOM	1	C	GLY	1	42.069	47.090	53.319	1.00	41.82
ATOM	2	O	GLY	1	42.192	48.313	53.390	1.00	43.35
ATOM	3	HT1	GLY	1	41.201	48.096	55.578	1.00	0.00
ATOM	4	HT2	GLY	1	40.002	46.972	56.021	1.00	0.00
ATOM	5	N	GLY	1	40.527	47.383	55.225	1.00	42.06
ATOM	6	HT3	GLY	1	39.884	47.885	54.576	1.00	0.00
ATOM	7	CA	GLY	1	41.301	46.401	54.465	1.00	41.76
ATOM	8	N	VAL	2	42.600	46.396	52.305	1.00	38.51
ATOM	9	H	VAL	2	42.552	45.423	52.352	1.00	0.00
ATOM	10	CA	VAL	2	43.257	47.052	51.168	1.00	36.15
ATOM	11	CB	VAL	2	44.072	45.930	50.446	1.00	35.20
ATOM	12	CG1	VAL	2	43.160	44.784	50.162	1.00	36.74
ATOM	13	CG2	VAL	2	44.661	46.365	49.109	1.00	33.68
ATOM	14	C	VAL	2	42.327	47.815	50.219	1.00	36.38
ATOM	15	O	VAL	2	41.121	47.775	50.382	1.00	39.17
ATOM	16	N	GLN	3	42.780	48.580	49.247	1.00	35.98
ATOM	17	H	GLN	3	43.706	48.879	49.318	1.00	0.00
ATOM	18	CA	GLN	3	41.905	49.201	48.276	1.00	34.49
ATOM	19	CB	GLN	3	41.521	50.543	48.810	1.00	33.04
ATOM	20	CG	GLN	3	40.565	51.283	47.925	1.00	36.48
ATOM	21	CD	GLN	3	40.481	52.766	48.248	1.00	37.58
ATOM	22	OE1	GLN	3	41.243	53.348	49.007	1.00	39.56
ATOM	23	NE2	GLN	3	39.588	53.526	47.665	1.00	38.51
ATOM	24	HE21	GLN	3	39.638	54.450	47.971	1.00	0.00
ATOM	25	HE22	GLN	3	38.980	53.155	47.002	1.00	0.00
ATOM	26	C	GLN	3	42.622	49.341	46.933	1.00	35.68
ATOM	27	O	GLN	3	43.488	50.208	46.802	1.00	36.78
ATOM	28	N	VAL	4	42.383	48.542	45.895	1.00	35.37
ATOM	29	H	VAL	4	41.698	47.845	45.965	1.00	0.00
ATOM	30	CA	VAL	4	43.090	48.778	44.637	1.00	36.52
ATOM	31	CB	VAL	4	43.088	47.481	43.779	1.00	37.20
ATOM	32	CG1	VAL	4	43.757	46.372	44.574	1.00	37.93
ATOM	33	CG2	VAL	4	41.679	47.004	43.446	1.00	38.64
ATOM	34	C	VAL	4	42.561	49.958	43.799	1.00	37.11
ATOM	35	O	VAL	4	41.453	49.956	43.272	1.00	37.77
ATOM	36	N	GLU	5	43.247	51.096	43.769	1.00	38.01
ATOM	37	H	GLU	5	43.922	51.237	44.467	1.00	0.00
ATOM	38	CA	GLU	5	42.900	52.179	42.850	1.00	38.19
ATOM	39	CB	GLU	5	42.971	53.497	43.620	1.00	41.44
ATOM	40	CG	GLU	5	41.899	53.624	44.721	1.00	47.00
ATOM	41	CD	GLU	5	42.112	54.827	45.661	1.00	52.99

FIGURE 1 (CONT.)

ATOM	42	OE1	GLU	5	42.618	54.659	46.786	1.00	55.30
ATOM	43	OE2	GLU	5	41.773	55.949	45.274	1.00	54.87
ATOM	44	C	GLU	5	43.892	52.149	41.668	1.00	37.89
ATOM	45	O	GLU	5	45.087	52.367	41.866	1.00	38.08
ATOM	46	N	THR	6	43.586	51.840	40.396	1.00	37.45
ATOM	47	H	THR	6	42.645	51.760	40.135	1.00	0.00
ATOM	48	CA	THR	6	44.662	51.769	39.388	1.00	36.36
ATOM	49	CB	THR	6	44.306	51.055	38.091	1.00	35.22
ATOM	50	OG1	THR	6	43.348	51.821	37.361	1.00	34.96
ATOM	51	HG1	THR	6	43.544	52.769	37.301	1.00	0.00
ATOM	52	CG2	THR	6	43.783	49.683	38.407	1.00	34.83
ATOM	53	C	THR	6	45.242	53.070	38.883	1.00	36.03
ATOM	54	O	THR	6	44.588	54.102	38.779	1.00	34.37
ATOM	55	N	ILE	7	46.499	52.948	38.513	1.00	36.48
ATOM	56	H	ILE	7	46.960	52.142	38.779	1.00	0.00
ATOM	57	CA	ILE	7	47.244	54.056	37.929	1.00	37.99
ATOM	58	CB	ILE	7	48.602	54.186	38.696	1.00	37.09
ATOM	59	CG2	ILE	7	49.467	55.319	38.135	1.00	38.38
ATOM	60	CG1	ILE	7	48.261	54.424	40.161	1.00	35.33
ATOM	61	CD1	ILE	7	49.400	54.804	41.082	1.00	34.52
ATOM	62	C	ILE	7	47.459	53.888	36.424	1.00	37.49
ATOM	63	O	ILE	7	47.305	54.830	35.638	1.00	38.48
ATOM	64	N	SER	8	47.833	52.670	36.033	1.00	36.45
ATOM	65	H	SER	8	48.045	52.009	36.725	1.00	0.00
ATOM	66	CA	SER	8	48.013	52.366	34.625	1.00	36.97
ATOM	67	CB	SER	8	49.397	52.794	34.130	1.00	37.72
ATOM	68	OG	SER	8	50.501	52.013	34.581	1.00	40.69
ATOM	69	HG	SER	8	50.341	51.065	34.470	1.00	0.00
ATOM	70	C	SER	8	47.844	50.886	34.314	1.00	38.32
ATOM	71	O	SER	8	48.604	50.034	34.790	1.00	38.56
ATOM	72	N	PRO	9	46.890	50.543	33.438	1.00	38.11
ATOM	73	CD	PRO	9	46.866	50.980	32.051	1.00	37.29
ATOM	74	CA	PRO	9	45.961	49.429	33.579	1.00	36.59
ATOM	75	CB	PRO	9	44.831	49.866	32.701	1.00	37.13
ATOM	76	CG	PRO	9	45.389	50.912	31.735	1.00	37.10
ATOM	77	C	PRO	9	46.385	47.984	33.321	1.00	35.28
ATOM	78	O	PRO	9	45.867	47.090	33.970	1.00	36.36
ATOM	79	N	GLY	10	47.273	47.625	32.421	1.00	34.47
ATOM	80	H	GLY	10	47.711	48.307	31.881	1.00	0.00
ATOM	81	CA	GLY	10	47.651	46.211	32.284	1.00	35.42
ATOM	82	C	GLY	10	46.639	45.294	31.618	1.00	35.67
ATOM	83	O	GLY	10	45.510	45.768	31.475	1.00	36.52
ATOM	84	N	ASP	11	46.914	44.030	31.177	1.00	34.34
ATOM	85	H	ASP	11	47.784	43.636	31.398	1.00	0.00
ATOM	86	CA	ASP	11	45.867	43.287	30.451	1.00	32.77

3/145

FIGURE 1 (CONT.)

ATOM	87	CB	ASP	11	46.513	42.108	29.677	1.00	30.21
ATOM	88	CG	ASP	11	47.046	40.838	30.335	1.00	31.55
ATOM	89	OD1	ASP	11	46.983	40.669	31.539	1.00	32.36
ATOM	90	OD2	ASP	11	47.554	39.968	29.637	1.00	32.01
ATOM	91	C	ASP	11	44.654	42.778	31.246	1.00	33.67
ATOM	92	O	ASP	11	44.786	41.802	31.975	1.00	35.19
ATOM	93	N	GLY	12	43.433	43.342	31.200	1.00	33.12
ATOM	94	H	GLY	12	43.375	44.219	30.771	1.00	0.00
ATOM	95	CA	GLY	12	42.266	42.803	31.947	1.00	34.13
ATOM	96	C	GLY	12	41.949	41.274	31.936	1.00	34.14
ATOM	97	O	GLY	12	40.937	40.858	32.478	1.00	33.16
ATOM	98	N	ARG	13	42.796	40.420	31.334	1.00	34.05
ATOM	99	H	ARG	13	43.551	40.821	30.882	1.00	0.00
ATOM	100	CA	ARG	13	42.712	38.977	31.239	1.00	35.99
ATOM	101	CB	ARG	13	42.524	38.606	29.760	1.00	34.93
ATOM	102	CG	ARG	13	42.456	39.627	28.611	1.00	33.77
ATOM	103	CD	ARG	13	43.730	39.644	27.772	1.00	32.76
ATOM	104	NE	ARG	13	44.211	38.299	27.561	1.00	34.61
ATOM	105	HE	ARG	13	43.573	37.556	27.533	1.00	0.00
ATOM	106	CZ	ARG	13	45.501	38.029	27.382	1.00	38.10
ATOM	107	NH1	ARG	13	45.864	36.745	27.291	1.00	38.67
ATOM	108	HH11	ARG	13	45.168	36.028	27.331	1.00	0.00
ATOM	109	HH12	ARG	13	46.819	36.503	27.122	1.00	0.00
ATOM	110	NH2	ARG	13	46.427	38.995	27.254	1.00	38.28
ATOM	111	HH21	ARG	13	46.176	39.959	27.310	1.00	0.00
ATOM	112	HH22	ARG	13	47.382	38.735	27.112	1.00	0.00
ATOM	113	C	ARG	13	43.877	38.115	31.819	1.00	38.59
ATOM	114	O	ARG	13	44.115	36.954	31.409	1.00	41.28
ATOM	115	N	THR	14	44.731	38.612	32.722	1.00	38.83
ATOM	116	H	THR	14	44.706	39.581	32.876	1.00	0.00
ATOM	117	CA	THR	14	45.771	37.752	33.328	1.00	39.77
ATOM	118	CB	THR	14	47.090	37.720	32.545	1.00	39.64
ATOM	119	OG1	THR	14	46.838	37.843	31.156	1.00	39.49
ATOM	120	HG1	THR	14	46.165	37.205	30.877	1.00	0.00
ATOM	121	CG2	THR	14	47.796	36.419	32.791	1.00	40.29
ATOM	122	C	THR	14	46.182	38.103	34.763	1.00	40.74
ATOM	123	O	THR	14	47.022	38.936	35.124	1.00	40.39
ATOM	124	N	PHE	15	45.513	37.341	35.604	1.00	40.86
ATOM	125	H	PHE	15	44.954	36.630	35.237	1.00	0.00
ATOM	126	CA	PHE	15	45.598	37.474	37.049	1.00	39.72
ATOM	127	CB	PHE	15	44.169	37.443	37.576	1.00	36.40
ATOM	128	CG	PHE	15	43.358	38.645	37.143	1.00	35.33
ATOM	129	CD1	PHE	15	43.197	39.701	38.029	1.00	34.10
ATOM	130	CD2	PHE	15	42.730	38.664	35.889	1.00	37.08
ATOM	131	CE1	PHE	15	42.396	40.784	37.666	1.00	35.93

4/145

FIGURE 1 (CONT.)

ATOM	132	CE2	PHE	15	41.930	39.752	35.540	1.00	35.56
ATOM	133	CZ	PHE	15	41.762	40.810	36.428	1.00	34.80
ATOM	134	C	PHE	15	46.469	36.454	37.814	1.00	39.79
ATOM	135	O	PHE	15	46.649	35.294	37.382	1.00	39.27
ATOM	136	N	PRO	16	47.039	36.846	38.966	1.00	39.55
ATOM	137	CD	PRO	16	46.973	38.189	39.561	1.00	38.77
ATOM	138	CA	PRO	16	47.804	35.929	39.788	1.00	39.65
ATOM	139	CB	PRO	16	48.632	36.893	40.614	1.00	39.12
ATOM	140	CG	PRO	16	47.675	38.043	40.892	1.00	38.01
ATOM	141	C	PRO	16	46.862	34.996	40.562	1.00	40.78
ATOM	142	O	PRO	16	45.770	35.371	41.072	1.00	38.94
ATOM	143	N	LYS	17	47.239	33.714	40.554	1.00	38.87
ATOM	144	H	LYS	17	47.937	33.411	39.941	1.00	0.00
ATOM	145	CA	LYS	17	46.461	32.820	41.394	1.00	40.02
ATOM	146	CB	LYS	17	45.761	31.810	40.478	1.00	41.97
ATOM	147	CG	LYS	17	46.634	30.839	39.712	1.00	42.19
ATOM	148	CD	LYS	17	45.801	29.939	38.819	1.00	42.73
ATOM	149	CE	LYS	17	46.535	28.596	38.652	1.00	45.69
ATOM	150	NZ	LYS	17	47.837	28.725	37.991	1.00	45.59
ATOM	151	HZ1	LYS	17	48.255	27.785	37.851	1.00	0.00
ATOM	152	HZ2	LYS	17	48.464	29.300	38.588	1.00	0.00
ATOM	153	HZ3	LYS	17	47.711	29.192	37.070	1.00	0.00
ATOM	154	C	LYS	17	47.300	32.143	42.488	1.00	41.12
ATOM	155	O	LYS	17	48.536	32.184	42.447	1.00	42.33
ATOM	156	N	ARG	18	46.723	31.543	43.535	1.00	40.99
ATOM	157	H	ARG	18	45.748	31.490	43.555	1.00	0.00
ATOM	158	CA	ARG	18	47.526	30.951	44.600	1.00	39.94
ATOM	159	CB	ARG	18	46.614	30.325	45.605	1.00	39.82
ATOM	160	CG	ARG	18	46.198	28.894	45.299	1.00	43.90
ATOM	161	CD	ARG	18	45.130	28.438	46.280	1.00	46.69
ATOM	162	NE	ARG	18	45.626	28.253	47.631	1.00	46.26
ATOM	163	HE	ARG	18	46.008	27.385	47.874	1.00	0.00
ATOM	164	CZ	ARG	18	45.589	29.215	48.554	1.00	47.53
ATOM	165	NH1	ARG	18	46.054	28.912	49.759	1.00	48.01
ATOM	166	HH11	ARG	18	46.414	27.999	49.943	1.00	0.00
ATOM	167	HH12	ARG	18	46.050	29.606	50.479	1.00	0.00
ATOM	168	NH2	ARG	18	45.128	30.452	48.294	1.00	48.91
ATOM	169	HH21	ARG	18	44.781	30.688	47.387	1.00	0.00
ATOM	170	HH22	ARG	18	45.121	31.140	49.020	1.00	0.00
ATOM	171	C	ARG	18	48.566	29.924	44.142	1.00	39.96
ATOM	172	O	ARG	18	48.407	29.161	43.181	1.00	38.95
ATOM	173	N	GLY	19	49.714	30.133	44.789	1.00	39.66
ATOM	174	H	GLY	19	49.729	30.840	45.455	1.00	0.00
ATOM	175	CA	GLY	19	50.931	29.369	44.547	1.00	37.93
ATOM	176	C	GLY	19	51.777	30.013	43.461	1.00	37.60

5/145

FIGURE 1 (CONT.)

ATOM	177	O	GLY	19	52.922	29.611	43.225	1.00	38.81
ATOM	178	N	GLN	20	51.199	31.031	42.792	1.00	35.56
ATOM	179	H	GLN	20	50.274	31.263	42.998	1.00	0.00
ATOM	180	CA	GLN	20	51.869	31.780	41.735	1.00	32.71
ATOM	181	CB	GLN	20	50.882	32.504	40.865	1.00	33.74
ATOM	182	CG	GLN	20	51.338	32.512	39.434	1.00	36.20
ATOM	183	CD	GLN	20	50.326	31.797	38.574	1.00	35.51
ATOM	184	OE1	GLN	20	49.681	32.411	37.739	1.00	36.56
ATOM	185	NE2	GLN	20	50.075	30.509	38.749	1.00	34.62
ATOM	186	HE21	GLN	20	50.536	29.998	39.437	1.00	0.00
ATOM	187	HE22	GLN	20	49.407	30.171	38.127	1.00	0.00
ATOM	188	C	GLN	20	52.832	32.830	42.204	1.00	30.13
ATOM	189	O	GLN	20	52.399	33.714	42.960	1.00	28.75
ATOM	190	N	THR	21	54.076	32.784	41.704	1.00	28.40
ATOM	191	H	THR	21	54.316	32.069	41.073	1.00	0.00
ATOM	192	CA	THR	21	55.067	33.801	42.075	1.00	26.74
ATOM	193	CB	THR	21	56.514	33.354	41.670	1.00	29.08
ATOM	194	OG1	THR	21	56.762	32.109	42.319	1.00	28.19
ATOM	195	HG1	THR	21	56.664	31.409	41.657	1.00	0.00
ATOM	196	CG2	THR	21	57.609	34.331	42.100	1.00	27.45
ATOM	197	C	THR	21	54.797	35.186	41.470	1.00	25.93
ATOM	198	O	THR	21	55.098	35.430	40.304	1.00	23.14
ATOM	199	N	CYS	22	54.154	36.112	42.202	1.00	27.31
ATOM	200	H	CYS	22	53.779	35.806	43.055	1.00	0.00
ATOM	201	CA	CYS	22	53.937	37.501	41.753	1.00	29.39
ATOM	202	CB	CYS	22	52.899	38.281	42.549	1.00	28.95
ATOM	203	SG	CYS	22	51.357	37.402	42.845	1.00	31.42
ATOM	204	C	CYS	22	55.162	38.426	41.811	1.00	30.45
ATOM	205	O	CYS	22	55.578	38.922	42.871	1.00	29.88
ATOM	206	N	VAL	23	55.774	38.632	40.634	1.00	30.12
ATOM	207	H	VAL	23	55.413	38.174	39.846	1.00	0.00
ATOM	208	CA	VAL	23	56.898	39.547	40.507	1.00	27.94
ATOM	209	CB	VAL	23	57.733	39.242	39.268	1.00	26.58
ATOM	210	CG1	VAL	23	59.047	39.982	39.453	1.00	23.51
ATOM	211	CG2	VAL	23	57.989	37.753	39.067	1.00	25.36
ATOM	212	C	VAL	23	56.359	40.980	40.389	1.00	27.94
ATOM	213	O	VAL	23	55.593	41.279	39.485	1.00	29.74
ATOM	214	N	VAL	24	56.635	41.873	41.322	1.00	26.11
ATOM	215	H	VAL	24	57.138	41.554	42.101	1.00	0.00
ATOM	216	CA	VAL	24	56.212	43.262	41.279	1.00	25.02
ATOM	217	CB	VAL	24	55.146	43.661	42.348	1.00	26.06
ATOM	218	CG1	VAL	24	53.762	43.087	42.093	1.00	25.35
ATOM	219	CG2	VAL	24	55.665	43.142	43.688	1.00	28.24
ATOM	220	C	VAL	24	57.393	44.185	41.569	1.00	25.29
ATOM	221	O	VAL	24	58.481	43.812	42.037	1.00	25.98

6/145

FIGURE 1 (CONT.)

ATOM	222	N	HIS	25	57.197	45.454	41.276	1.00	21.24
ATOM	223	H	HIS	25	56.376	45.706	40.791	1.00	0.00
ATOM	224	CA	HIS	25	58.146	46.421	41.707	1.00	21.30
ATOM	225	CB	HIS	25	58.736	47.210	40.563	1.00	26.13
ATOM	226	CG	HIS	25	60.271	47.203	40.531	1.00	28.07
ATOM	227	CD2	HIS	25	60.974	47.708	39.475	1.00	29.42
ATOM	228	ND1	HIS	25	61.198	46.773	41.390	1.00	29.32
ATOM	229	HD1	HIS	25	61.047	46.384	42.281	1.00	0.00
ATOM	230	CE1	HIS	25	62.384	46.994	40.915	1.00	27.59
ATOM	231	NE2	HIS	25	62.239	47.559	39.760	1.00	28.50
ATOM	232	HE2	HIS	25	62.985	47.893	39.210	1.00	0.00
ATOM	233	C	HIS	25	57.236	47.303	42.508	1.00	23.00
ATOM	234	O	HIS	25	56.236	47.738	41.970	1.00	26.21
ATOM	235	N	TYR	26	57.454	47.566	43.784	1.00	20.88
ATOM	236	H	TYR	26	58.222	47.138	44.208	1.00	0.00
ATOM	237	CA	TYR	26	56.544	48.416	44.538	1.00	18.89
ATOM	238	CB	TYR	26	56.068	47.697	45.797	1.00	17.38
ATOM	239	CG	TYR	26	57.155	47.348	46.802	1.00	15.80
ATOM	240	CD1	TYR	26	57.447	48.208	47.877	1.00	14.23
ATOM	241	CE1	TYR	26	58.468	47.879	48.774	1.00	11.98
ATOM	242	CD2	TYR	26	57.886	46.157	46.621	1.00	16.82
ATOM	243	CE2	TYR	26	58.917	45.840	47.511	1.00	15.75
ATOM	244	CZ	TYR	26	59.187	46.706	48.582	1.00	14.95
ATOM	245	OH	TYR	26	60.174	46.341	49.466	1.00	20.01
ATOM	246	HH	TYR	26	59.987	46.721	50.340	1.00	0.00
ATOM	247	C	TYR	26	57.152	49.730	44.979	1.00	19.71
ATOM	248	O	TYR	26	58.355	49.948	44.830	1.00	23.57
ATOM	249	N	THR	27	56.347	50.586	45.567	1.00	19.61
ATOM	250	H	THR	27	55.385	50.494	45.384	1.00	0.00
ATOM	251	CA	THR	27	56.823	51.753	46.301	1.00	20.40
ATOM	252	CB	THR	27	57.006	53.035	45.434	1.00	21.63
ATOM	253	OG1	THR	27	58.193	52.798	44.677	1.00	20.88
ATOM	254	HG1	THR	27	57.901	52.431	43.834	1.00	0.00
ATOM	255	CG2	THR	27	57.186	54.335	46.231	1.00	18.41
ATOM	256	C	THR	27	55.834	52.083	47.404	1.00	19.02
ATOM	257	O	THR	27	54.721	52.526	47.190	1.00	19.18
ATOM	258	N	GLY	28	56.236	51.771	48.612	1.00	20.92
ATOM	259	H	GLY	28	57.161	51.471	48.732	1.00	0.00
ATOM	260	CA	GLY	28	55.436	52.035	49.785	1.00	23.65
ATOM	261	C	GLY	28	55.701	53.389	50.432	1.00	26.52
ATOM	262	O	GLY	28	56.822	53.926	50.550	1.00	27.81
ATOM	263	N	MET	29	54.567	53.921	50.871	1.00	27.75
ATOM	264	H	MET	29	53.725	53.435	50.718	1.00	0.00
ATOM	265	CA	MET	29	54.491	55.225	51.510	1.00	27.83
ATOM	266	CB	MET	29	53.905	56.309	50.650	1.00	30.08

7/145

FIGURE 1 (CONT.)

ATOM	267	CG	MET	29	54.666	56.679	49.419	1.00	32.75
ATOM	268	SD	MET	29	53.495	56.923	48.087	1.00	34.24
ATOM	269	CE	MET	29	54.295	55.650	47.175	1.00	35.09
ATOM	270	C	MET	29	53.538	55.177	52.658	1.00	27.17
ATOM	271	O	MET	29	52.720	54.267	52.817	1.00	26.91
ATOM	272	N	LEU	30	53.677	56.181	53.490	1.00	27.89
ATOM	273	H	LEU	30	54.483	56.732	53.446	1.00	0.00
ATOM	274	CA	LEU	30	52.667	56.356	54.516	1.00	30.48
ATOM	275	CB	LEU	30	53.298	57.017	55.777	1.00	27.96
ATOM	276	CG	LEU	30	54.527	56.394	56.423	1.00	25.12
ATOM	277	CD1	LEU	30	55.041	57.364	57.456	1.00	23.11
ATOM	278	CD2	LEU	30	54.204	55.058	57.065	1.00	21.88
ATOM	279	C	LEU	30	51.524	57.228	53.941	1.00	31.36
ATOM	280	O	LEU	30	51.602	57.856	52.863	1.00	29.62
ATOM	281	N	GLU	31	50.441	57.323	54.702	1.00	31.29
ATOM	282	H	GLU	31	50.378	56.747	55.493	1.00	0.00
ATOM	283	CA	GLU	31	49.262	58.044	54.236	1.00	32.84
ATOM	284	CB	GLU	31	48.178	57.796	55.298	1.00	32.44
ATOM	285	CG	GLU	31	46.770	58.072	54.796	1.00	31.53
ATOM	286	CD	GLU	31	45.698	57.826	55.833	1.00	34.07
ATOM	287	OE1	GLU	31	44.549	57.608	55.422	1.00	34.66
ATOM	288	OE2	GLU	31	46.013	57.857	57.036	1.00	33.21
ATOM	289	C	GLU	31	49.441	59.535	53.905	1.00	32.14
ATOM	290	O	GLU	31	48.616	60.173	53.260	1.00	33.96
ATOM	291	N	ASP	32	50.540	60.143	54.310	1.00	31.59
ATOM	292	H	ASP	32	51.134	59.673	54.927	1.00	0.00
ATOM	293	CA	ASP	32	50.783	61.517	53.895	1.00	31.09
ATOM	294	CB	ASP	32	51.608	62.280	54.938	1.00	32.37
ATOM	295	CG	ASP	32	52.895	61.673	55.492	1.00	33.17
ATOM	296	OD1	ASP	32	53.434	62.267	56.421	1.00	35.90
ATOM	297	OD2	ASP	32	53.350	60.626	55.044	1.00	33.02
ATOM	298	C	ASP	32	51.496	61.601	52.570	1.00	31.07
ATOM	299	O	ASP	32	51.721	62.674	52.022	1.00	34.08
ATOM	300	N	GLY	33	51.843	60.432	52.042	1.00	31.65
ATOM	301	H	GLY	33	51.444	59.632	52.417	1.00	0.00
ATOM	302	CA	GLY	33	52.607	60.313	50.802	1.00	30.10
ATOM	303	C	GLY	33	54.090	60.071	51.065	1.00	29.11
ATOM	304	O	GLY	33	54.873	59.762	50.168	1.00	30.34
ATOM	305	N	LYS	34	54.563	60.167	52.305	1.00	28.54
ATOM	306	H	LYS	34	53.959	60.458	53.009	1.00	0.00
ATOM	307	CA	LYS	34	55.984	59.971	52.538	1.00	28.12
ATOM	308	CB	LYS	34	56.360	60.398	53.936	1.00	28.68
ATOM	309	CG	LYS	34	57.865	60.568	54.117	1.00	27.68
ATOM	310	CD	LYS	34	58.081	61.183	55.479	1.00	28.13
ATOM	311	CE	LYS	34	57.705	60.187	56.545	1.00	27.71

FIGURE 1 (CONT.)

ATOM	312	NZ	LYS	34	58.191	60.672	57.813	1.00	29.87
ATOM	313	HZ1	LYS	34	57.696	61.553	58.056	1.00	0.00
ATOM	314	HZ2	LYS	34	59.213	60.854	57.752	1.00	0.00
ATOM	315	HZ3	LYS	34	58.008	59.959	58.547	1.00	0.00
ATOM	316	C	LYS	34	56.496	58.555	52.335	1.00	27.80
ATOM	317	O	LYS	34	56.101	57.581	52.991	1.00	30.02
ATOM	318	N	LYS	35	57.347	58.486	51.323	1.00	25.28
ATOM	319	H	LYS	35	57.412	59.266	50.737	1.00	0.00
ATOM	320	CA	LYS	35	58.062	57.274	51.007	1.00	23.24
ATOM	321	CB	LYS	35	59.032	57.523	49.855	1.00	18.81
ATOM	322	CG	LYS	35	59.361	56.174	49.209	1.00	18.77
ATOM	323	CD	LYS	35	60.466	56.193	48.143	1.00	17.00
ATOM	324	CE	LYS	35	61.856	56.062	48.750	1.00	16.60
ATOM	325	NZ	LYS	35	62.806	55.735	47.710	1.00	18.86
ATOM	326	HZ1	LYS	35	62.765	56.447	46.952	1.00	0.00
ATOM	327	HZ2	LYS	35	62.576	54.799	47.323	1.00	0.00
ATOM	328	HZ3	LYS	35	63.760	55.721	48.122	1.00	0.00
ATOM	329	C	LYS	35	58.841	56.759	52.214	1.00	23.19
ATOM	330	O	LYS	35	59.441	57.506	52.993	1.00	25.70
ATOM	331	N	PHE	36	58.677	55.471	52.433	1.00	21.46
ATOM	332	H	PHE	36	57.956	55.019	51.940	1.00	0.00
ATOM	333	CA	PHE	36	59.442	54.770	53.439	1.00	18.53
ATOM	334	CB	PHE	36	58.557	54.038	54.487	1.00	15.06
ATOM	335	CG	PHE	36	57.485	53.000	54.092	1.00	15.47
ATOM	336	CD1	PHE	36	56.127	53.322	54.281	1.00	11.31
ATOM	337	CD2	PHE	36	57.829	51.703	53.619	1.00	15.12
ATOM	338	CE1	PHE	36	55.134	52.362	54.006	1.00	12.76
ATOM	339	CE2	PHE	36	56.820	50.760	53.346	1.00	15.65
ATOM	340	CZ	PHE	36	55.466	51.083	53.543	1.00	9.65
ATOM	341	C	PHE	36	60.288	53.752	52.720	1.00	20.38
ATOM	342	O	PHE	36	61.377	53.520	53.205	1.00	24.97
ATOM	343	N	ASP	37	59.909	53.117	51.594	1.00	19.98
ATOM	344	H	ASP	37	59.015	53.280	51.221	1.00	0.00
ATOM	345	CA	ASP	37	60.786	52.151	50.924	1.00	19.12
ATOM	346	CB	ASP	37	60.755	50.796	51.671	1.00	21.95
ATOM	347	CG	ASP	37	61.641	49.636	51.198	1.00	21.09
ATOM	348	OD1	ASP	37	61.238	48.497	51.386	1.00	22.65
ATOM	349	OD2	ASP	37	62.722	49.847	50.660	1.00	22.17
ATOM	350	C	ASP	37	60.350	51.925	49.495	1.00	17.87
ATOM	351	O	ASP	37	59.294	52.376	49.117	1.00	17.69
ATOM	352	N	SER	38	61.118	51.231	48.678	1.00	17.89
ATOM	353	H	SER	38	62.003	50.983	49.010	1.00	0.00
ATOM	354	CA	SER	38	60.779	50.896	47.310	1.00	17.18
ATOM	355	CB	SER	38	60.908	52.048	46.328	1.00	18.01
ATOM	356	OG	SER	38	60.771	51.662	44.958	1.00	19.28

9/145

FIGURE 1 (CONT.)

ATOM	357	HG	SER	38	59.971	52.126	44.651	1.00	0.00
ATOM	358	C	SER	38	61.705	49.845	46.765	1.00	17.77
ATOM	359	O	SER	38	62.911	49.958	46.948	1.00	20.48
ATOM	360	N	SER	39	61.213	48.833	46.051	1.00	16.66
ATOM	361	H	SER	39	60.238	48.777	46.012	1.00	0.00
ATOM	362	CA	SER	39	62.071	47.849	45.366	1.00	17.42
ATOM	363	CB	SER	39	61.223	46.796	44.704	1.00	15.25
ATOM	364	OG	SER	39	60.344	47.446	43.781	1.00	16.64
ATOM	365	HG	SER	39	59.996	48.275	44.158	1.00	0.00
ATOM	366	C	SER	39	62.986	48.430	44.279	1.00	20.01
ATOM	367	O	SER	39	63.897	47.810	43.721	1.00	19.70
ATOM	368	N	ARG	40	62.679	49.672	43.907	1.00	23.62
ATOM	369	H	ARG	40	61.914	50.125	44.324	1.00	0.00
ATOM	370	CA	ARG	40	63.425	50.443	42.916	1.00	25.92
ATOM	371	CB	ARG	40	62.541	51.567	42.399	1.00	22.84
ATOM	372	CG	ARG	40	61.420	51.048	41.552	1.00	22.60
ATOM	373	CD	ARG	40	60.536	52.150	40.979	1.00	25.68
ATOM	374	NE	ARG	40	59.457	51.564	40.188	1.00	31.06
ATOM	375	HE	ARG	40	58.539	51.609	40.524	1.00	0.00
ATOM	376	CZ	ARG	40	59.704	50.930	39.010	1.00	34.77
ATOM	377	NH1	ARG	40	58.669	50.342	38.376	1.00	31.00
ATOM	378	HH11	ARG	40	57.759	50.363	38.788	1.00	0.00
ATOM	379	HH12	ARG	40	58.825	49.854	37.517	1.00	0.00
ATOM	380	NH2	ARG	40	60.955	50.885	38.457	1.00	32.96
ATOM	381	HH21	ARG	40	61.724	51.332	38.913	1.00	0.00
ATOM	382	HH22	ARG	40	61.098	50.408	37.590	1.00	0.00
ATOM	383	C	ARG	40	64.724	51.018	43.469	1.00	27.43
ATOM	384	O	ARG	40	65.693	51.163	42.728	1.00	29.93
ATOM	385	N	ASP	41	64.764	51.230	44.800	1.00	27.19
ATOM	386	H	ASP	41	63.924	51.110	45.289	1.00	0.00
ATOM	387	CA	ASP	41	65.928	51.717	45.559	1.00	24.84
ATOM	388	CB	ASP	41	65.696	51.745	47.061	1.00	21.53
ATOM	389	CG	ASP	41	64.640	52.675	47.624	1.00	21.05
ATOM	390	OD1	ASP	41	64.413	52.612	48.832	1.00	20.59
ATOM	391	OD2	ASP	41	64.051	53.459	46.880	1.00	23.80
ATOM	392	C	ASP	41	67.177	50.870	45.400	1.00	24.97
ATOM	393	O	ASP	41	68.345	51.283	45.514	1.00	25.61
ATOM	394	N	ARG	42	66.830	49.603	45.245	1.00	22.10
ATOM	395	H	ARG	42	65.887	49.361	45.318	1.00	0.00
ATOM	396	CA	ARG	42	67.850	48.604	45.080	1.00	22.23
ATOM	397	CB	ARG	42	67.791	47.652	46.309	1.00	21.91
ATOM	398	CG	ARG	42	66.432	47.150	46.667	1.00	23.04
ATOM	399	CD	ARG	42	66.300	46.343	47.924	1.00	20.28
ATOM	400	NE	ARG	42	64.947	45.806	47.920	1.00	14.87
ATOM	401	HE	ARG	42	64.807	44.872	47.657	1.00	0.00

10/145

FIGURE 1 (CONT.)

ATOM	402	CZ	ARG	42	63.895	46.531	48.275	1.00	13.69
ATOM	403	NH1	ARG	42	62.703	45.970	48.215	1.00	17.94
ATOM	404	HH11	ARG	42	62.607	45.021	47.917	1.00	0.00
ATOM	405	HH12	ARG	42	61.894	46.497	48.472	1.00	0.00
ATOM	406	NH2	ARG	42	63.992	47.759	48.747	1.00	12.98
ATOM	407	HH21	ARG	42	64.888	48.190	48.860	1.00	0.00
ATOM	408	HH22	ARG	42	63.166	48.265	48.999	1.00	0.00
ATOM	409	C	ARG	42	67.706	47.882	43.758	1.00	21.35
ATOM	410	O	ARG	42	68.304	46.846	43.489	1.00	21.41
ATOM	411	N	ASN	43	66.954	48.520	42.872	1.00	22.88
ATOM	412	H	ASN	43	66.681	49.440	43.070	1.00	0.00
ATOM	413	CA	ASN	43	66.663	47.970	41.559	1.00	24.51
ATOM	414	CB	ASN	43	67.796	48.385	40.679	1.00	24.48
ATOM	415	CG	ASN	43	67.440	49.794	40.271	1.00	29.50
ATOM	416	OD1	ASN	43	66.386	49.982	39.670	1.00	33.59
ATOM	417	ND2	ASN	43	68.178	50.852	40.553	1.00	27.08
ATOM	418	HD21	ASN	43	67.776	51.686	40.250	1.00	0.00
ATOM	419	HD22	ASN	43	69.016	50.738	41.032	1.00	0.00
ATOM	420	C	ASN	43	66.390	46.479	41.424	1.00	24.85
ATOM	421	O	ASN	43	66.762	45.855	40.438	1.00	27.39
ATOM	422	N	LYS	44	65.709	45.900	42.419	1.00	24.30
ATOM	423	H	LYS	44	65.401	46.462	43.161	1.00	0.00
ATOM	424	CA	LYS	44	65.426	44.470	42.473	1.00	23.99
ATOM	425	CB	LYS	44	65.808	43.933	43.792	1.00	20.96
ATOM	426	CG	LYS	44	66.506	42.628	43.684	1.00	23.46
ATOM	427	CD	LYS	44	67.863	42.872	43.144	1.00	23.83
ATOM	428	CE	LYS	44	68.256	41.581	42.481	1.00	27.20
ATOM	429	NZ	LYS	44	68.729	40.675	43.507	1.00	36.28
ATOM	430	HZ1	LYS	44	69.086	39.801	43.071	1.00	0.00
ATOM	431	HZ2	LYS	44	67.963	40.456	44.175	1.00	0.00
ATOM	432	HZ3	LYS	44	69.502	41.148	44.020	1.00	0.00
ATOM	433	C	LYS	44	63.941	44.274	42.312	1.00	27.07
ATOM	434	O	LYS	44	63.200	44.934	43.055	1.00	31.31
ATOM	435	N	PRO	45	63.332	43.560	41.365	1.00	28.67
ATOM	436	CD	PRO	45	63.807	43.335	40.005	1.00	28.62
ATOM	437	CA	PRO	45	61.909	43.224	41.470	1.00	28.69
ATOM	438	CB	PRO	45	61.624	42.545	40.166	1.00	26.52
ATOM	439	CG	PRO	45	62.484	43.360	39.229	1.00	27.83
ATOM	440	C	PRO	45	61.617	42.379	42.708	1.00	27.51
ATOM	441	O	PRO	45	62.368	41.468	43.045	1.00	29.13
ATOM	442	N	PHE	46	60.597	42.725	43.452	1.00	26.12
ATOM	443	H	PHE	46	60.007	43.450	43.168	1.00	0.00
ATOM	444	CA	PHE	46	60.248	41.920	44.597	1.00	31.28
ATOM	445	CB	PHE	46	59.465	42.716	45.650	1.00	32.61
ATOM	446	CG	PHE	46	59.120	41.920	46.901	1.00	33.87

11/145

FIGURE 1 (CONT.)

ATOM	447	CD1	PHE	46	57.828	41.384	47.059	1.00	37.56
ATOM	448	CD2	PHE	46	60.082	41.724	47.893	1.00	33.24
ATOM	449	CE1	PHE	46	57.510	40.654	48.212	1.00	35.56
ATOM	450	CE2	PHE	46	59.752	40.996	49.036	1.00	31.96
ATOM	451	CZ	PHE	46	58.479	40.465	49.195	1.00	34.08
ATOM	452	C	PHE	46	59.359	40.785	44.127	1.00	34.32
ATOM	453	O	PHE	46	58.313	41.026	43.503	1.00	36.16
ATOM	454	N	LYS	47	59.737	39.552	44.453	1.00	33.97
ATOM	455	H	LYS	47	60.573	39.430	44.943	1.00	0.00
ATOM	456	CA	LYS	47	58.898	38.431	44.081	1.00	33.67
ATOM	457	CB	LYS	47	59.676	37.387	43.326	1.00	32.98
ATOM	458	CG	LYS	47	60.550	37.818	42.159	1.00	33.56
ATOM	459	CD	LYS	47	61.116	36.562	41.503	1.00	36.93
ATOM	460	CE	LYS	47	61.795	35.672	42.568	1.00	42.30
ATOM	461	NZ	LYS	47	61.538	34.243	42.355	1.00	47.07
ATOM	462	HZ1	LYS	47	62.041	33.696	43.081	1.00	0.00
ATOM	463	HZ2	LYS	47	61.876	33.968	41.411	1.00	0.00
ATOM	464	HZ3	LYS	47	60.517	34.060	42.431	1.00	0.00
ATOM	465	C	LYS	47	58.297	37.745	45.295	1.00	34.78
ATOM	466	O	LYS	47	58.927	37.710	46.354	1.00	35.77
ATOM	467	N	PHE	48	57.064	37.230	45.188	1.00	36.45
ATOM	468	H	PHE	48	56.529	37.505	44.412	1.00	0.00
ATOM	469	CA	PHE	48	56.428	36.398	46.226	1.00	34.29
ATOM	470	CB	PHE	48	55.710	37.268	47.252	1.00	30.97
ATOM	471	CG	PHE	48	54.509	38.048	46.766	1.00	31.16
ATOM	472	CD1	PHE	48	54.679	39.206	46.001	1.00	30.30
ATOM	473	CD2	PHE	48	53.212	37.643	47.146	1.00	32.81
ATOM	474	CE1	PHE	48	53.545	39.949	45.634	1.00	31.75
ATOM	475	CE2	PHE	48	52.085	38.402	46.770	1.00	29.93
ATOM	476	CZ	PHE	48	52.254	39.557	46.016	1.00	29.15
ATOM	477	C	PHE	48	55.414	35.364	45.707	1.00	34.91
ATOM	478	O	PHE	48	54.771	35.615	44.697	1.00	35.21
ATOM	479	N	MET	49	55.293	34.189	46.341	1.00	35.75
ATOM	480	H	MET	49	55.922	34.053	47.077	1.00	0.00
ATOM	481	CA	MET	49	54.326	33.108	46.087	1.00	35.33
ATOM	482	CB	MET	49	54.925	31.803	46.679	1.00	38.16
ATOM	483	CG	MET	49	54.063	30.523	46.688	1.00	45.74
ATOM	484	SD	MET	49	54.317	29.195	47.950	1.00	53.12
ATOM	485	CE	MET	49	55.717	28.211	47.465	1.00	47.62
ATOM	486	C	MET	49	52.951	33.437	46.718	1.00	34.27
ATOM	487	O	MET	49	52.802	33.406	47.946	1.00	35.14
ATOM	488	N	LEU	50	51.906	33.818	45.956	1.00	33.74
ATOM	489	H	LEU	50	52.087	33.902	44.992	1.00	0.00
ATOM	490	CA	LEU	50	50.544	34.145	46.466	1.00	30.96
ATOM	491	CB	LEU	50	49.704	34.589	45.273	1.00	28.85

12/145

FIGURE 1 (CONT.)

ATOM	492	CG	LEU	50	48.364	35.276	45.440	1.00	26.99
ATOM	493	CD1	LEU	50	48.504	36.547	46.254	1.00	27.85
ATOM	494	CD2	LEU	50	47.842	35.636	44.088	1.00	22.86
ATOM	495	C	LEU	50	49.808	33.018	47.226	1.00	32.10
ATOM	496	O	LEU	50	50.064	31.831	46.968	1.00	33.28
ATOM	497	N	GLY	51	48.875	33.204	48.170	1.00	32.19
ATOM	498	H	GLY	51	48.557	34.116	48.321	1.00	0.00
ATOM	499	CA	GLY	51	48.310	32.048	48.914	1.00	32.20
ATOM	500	C	GLY	51	49.144	31.575	50.118	1.00	32.53
ATOM	501	O	GLY	51	48.692	31.520	51.253	1.00	30.27
ATOM	502	N	LYS	52	50.419	31.279	49.905	1.00	35.99
ATOM	503	H	LYS	52	50.712	31.268	48.971	1.00	0.00
ATOM	504	CA	LYS	52	51.397	30.935	50.944	1.00	37.12
ATOM	505	CB	LYS	52	52.654	30.449	50.251	1.00	41.85
ATOM	506	CG	LYS	52	53.557	29.560	51.117	1.00	47.92
ATOM	507	CD	LYS	52	55.001	30.068	51.090	1.00	50.14
ATOM	508	CE	LYS	52	55.671	29.809	52.438	1.00	52.41
ATOM	509	NZ	LYS	52	57.050	30.246	52.362	1.00	55.15
ATOM	510	HZ1	LYS	52	57.521	30.087	53.275	1.00	0.00
ATOM	511	HZ2	LYS	52	57.050	31.264	52.148	1.00	0.00
ATOM	512	HZ3	LYS	52	57.555	29.735	51.612	1.00	0.00
ATOM	513	C	LYS	52	51.786	32.005	51.974	1.00	35.55
ATOM	514	O	LYS	52	52.895	32.040	52.474	1.00	35.47
ATOM	515	N	GLN	53	50.965	32.970	52.378	1.00	36.40
ATOM	516	H	GLN	53	50.055	32.946	52.017	1.00	0.00
ATOM	517	CA	GLN	53	51.294	33.898	53.479	1.00	37.96
ATOM	518	CB	GLN	53	51.170	33.090	54.792	1.00	40.53
ATOM	519	CG	GLN	53	50.001	32.088	54.980	1.00	44.03
ATOM	520	CD	GLN	53	50.479	30.689	55.421	1.00	43.54
ATOM	521	OE1	GLN	53	50.412	29.683	54.711	1.00	41.92
ATOM	522	NE2	GLN	53	51.030	30.534	56.611	1.00	43.08
ATOM	523	HE21	GLN	53	51.286	29.611	56.795	1.00	0.00
ATOM	524	HE22	GLN	53	51.156	31.307	57.188	1.00	0.00
ATOM	525	C	GLN	53	52.624	34.715	53.523	1.00	38.13
ATOM	526	O	GLN	53	52.994	35.274	54.560	1.00	39.71
ATOM	527	N	GLU	54	53.443	34.841	52.474	1.00	37.00
ATOM	528	H	GLU	54	53.262	34.222	51.741	1.00	0.00
ATOM	529	CA	GLU	54	54.709	35.618	52.489	1.00	36.22
ATOM	530	CB	GLU	54	55.472	35.223	51.222	1.00	36.71
ATOM	531	CG	GLU	54	55.891	33.753	51.070	1.00	36.14
ATOM	532	CD	GLU	54	56.704	33.442	49.817	1.00	38.51
ATOM	533	OE1	GLU	54	57.119	34.382	49.126	1.00	38.90
ATOM	534	OE2	GLU	54	56.928	32.258	49.523	1.00	39.98
ATOM	535	C	GLU	54	54.741	37.184	52.627	1.00	35.40
ATOM	536	O	GLU	54	55.771	37.873	52.686	1.00	35.37

13/145

FIGURE 1 (CONT.)

ATOM	537	N	VAL	55	53.587	37.844	52.632	1.00	33.24
ATOM	538	H	VAL	55	52.773	37.305	52.699	1.00	0.00
ATOM	539	CA	VAL	55	53.478	39.291	52.675	1.00	29.96
ATOM	540	CB	VAL	55	53.299	39.801	51.193	1.00	30.84
ATOM	541	CG1	VAL	55	54.436	39.323	50.303	1.00	29.50
ATOM	542	CG2	VAL	55	52.000	39.285	50.598	1.00	29.78
ATOM	543	C	VAL	55	52.303	39.761	53.570	1.00	29.32
ATOM	544	O	VAL	55	51.381	38.981	53.886	1.00	29.24
ATOM	545	N	ILE	56	52.244	41.021	54.005	1.00	28.85
ATOM	546	H	ILE	56	53.060	41.556	53.927	1.00	0.00
ATOM	547	CA	ILE	56	51.082	41.525	54.744	1.00	28.81
ATOM	548	CB	ILE	56	51.242	43.048	55.091	1.00	28.00
ATOM	549	CG2	ILE	56	52.228	43.047	56.234	1.00	28.05
ATOM	550	CG1	ILE	56	51.662	43.961	53.956	1.00	24.01
ATOM	551	CD1	ILE	56	51.316	45.414	54.287	1.00	17.23
ATOM	552	C	ILE	56	49.738	41.318	54.006	1.00	29.72
ATOM	553	O	ILE	56	49.735	41.387	52.769	1.00	30.04
ATOM	554	N	ARG	57	48.579	41.114	54.675	1.00	30.29
ATOM	555	H	ARG	57	48.601	41.193	55.657	1.00	0.00
ATOM	556	CA	ARG	57	47.371	40.689	53.974	1.00	31.47
ATOM	557	CB	ARG	57	46.365	40.215	54.974	1.00	32.72
ATOM	558	CG	ARG	57	45.411	39.104	54.490	1.00	38.09
ATOM	559	CD	ARG	57	45.981	37.653	54.488	1.00	41.25
ATOM	560	NE	ARG	57	44.951	36.602	54.311	1.00	45.34
ATOM	561	HE	ARG	57	44.950	36.114	53.462	1.00	0.00
ATOM	562	CZ	ARG	57	44.012	36.222	55.255	1.00	48.44
ATOM	563	NH1	ARG	57	43.125	35.237	54.974	1.00	44.33
ATOM	564	HH11	ARG	57	43.170	34.768	54.091	1.00	0.00
ATOM	565	HH12	ARG	57	42.458	34.951	55.662	1.00	0.00
ATOM	566	NH2	ARG	57	43.923	36.770	56.494	1.00	46.09
ATOM	567	HH21	ARG	57	43.215	36.452	57.124	1.00	0.00
ATOM	568	HH22	ARG	57	44.547	37.502	56.763	1.00	0.00
ATOM	569	C	ARG	57	46.754	41.751	53.093	1.00	32.82
ATOM	570	O	ARG	57	45.949	41.493	52.191	1.00	36.68
ATOM	571	N	GLY	58	47.191	42.983	53.321	1.00	32.92
ATOM	572	H	GLY	58	47.709	43.132	54.137	1.00	0.00
ATOM	573	CA	GLY	58	46.891	44.102	52.445	1.00	29.68
ATOM	574	C	GLY	58	47.551	43.795	51.119	1.00	29.05
ATOM	575	O	GLY	58	46.937	43.991	50.074	1.00	31.35
ATOM	576	N	TRP	59	48.765	43.241	51.093	1.00	28.03
ATOM	577	H	TRP	59	49.243	43.102	51.934	1.00	0.00
ATOM	578	CA	TRP	59	49.332	42.816	49.818	1.00	28.52
ATOM	579	CB	TRP	59	50.821	42.548	49.847	1.00	26.34
ATOM	580	CG	TRP	59	51.689	43.718	49.340	1.00	23.30
ATOM	581	CD2	TRP	59	52.739	43.650	48.445	1.00	17.27

FIGURE 1 (CONT.)

ATOM	582	CE2	TRP	59	53.247	44.928	48.520	1.00	15.62
ATOM	583	CE3	TRP	59	53.353	42.732	47.610	1.00	18.23
ATOM	584	CD1	TRP	59	51.551	44.963	49.887	1.00	20.47
ATOM	585	NE1	TRP	59	52.526	45.656	49.369	1.00	20.44
ATOM	586	HE1	TRP	59	52.604	46.626	49.499	1.00	0.00
ATOM	587	CZ2	TRP	59	54.356	45.312	47.792	1.00	14.10
ATOM	588	CZ3	TRP	59	54.476	43.104	46.865	1.00	16.40
ATOM	589	CH2	TRP	59	54.981	44.393	46.958	1.00	14.34
ATOM	590	C	TRP	59	48.745	41.555	49.240	1.00	29.75
ATOM	591	O	TRP	59	48.380	41.568	48.075	1.00	30.98
ATOM	592	N	GLU	60	48.575	40.458	49.963	1.00	33.00
ATOM	593	H	GLU	60	48.885	40.486	50.893	1.00	0.00
ATOM	594	CA	GLU	60	47.988	39.243	49.364	1.00	36.15
ATOM	595	CB	GLU	60	47.851	38.104	50.380	1.00	38.46
ATOM	596	CG	GLU	60	48.122	36.774	49.652	1.00	41.72
ATOM	597	CD	GLU	60	49.291	35.928	50.149	1.00	44.26
ATOM	598	OE1	GLU	60	49.063	34.762	50.479	1.00	45.57
ATOM	599	OE2	GLU	60	50.426	36.406	50.194	1.00	47.14
ATOM	600	C	GLU	60	46.616	39.443	48.744	1.00	37.17
ATOM	601	O	GLU	60	46.388	39.068	47.590	1.00	35.88
ATOM	602	N	GLU	61	45.721	40.094	49.492	1.00	38.28
ATOM	603	H	GLU	61	45.949	40.334	50.415	1.00	0.00
ATOM	604	CA	GLU	61	44.428	40.455	48.946	1.00	40.12
ATOM	605	CB	GLU	61	43.541	40.997	50.079	1.00	41.82
ATOM	606	CG	GLU	61	42.032	41.132	49.685	1.00	45.70
ATOM	607	CD	GLU	61	41.126	41.860	50.681	1.00	46.57
ATOM	608	OE1	GLU	61	41.018	41.378	51.816	1.00	48.32
ATOM	609	OE2	GLU	61	40.546	42.897	50.326	1.00	42.68
ATOM	610	C	GLU	61	44.545	41.513	47.806	1.00	40.85
ATOM	611	O	GLU	61	44.018	41.302	46.700	1.00	43.70
ATOM	612	N	GLY	62	45.256	42.643	47.983	1.00	38.17
ATOM	613	H	GLY	62	45.724	42.757	48.837	1.00	0.00
ATOM	614	CA	GLY	62	45.362	43.702	46.988	1.00	33.48
ATOM	615	C	GLY	62	45.998	43.311	45.661	1.00	32.00
ATOM	616	O	GLY	62	45.474	43.556	44.567	1.00	31.30
ATOM	617	N	VAL	63	47.154	42.680	45.733	1.00	30.37
ATOM	618	H	VAL	63	47.564	42.533	46.611	1.00	0.00
ATOM	619	CA	VAL	63	47.809	42.229	44.516	1.00	31.68
ATOM	620	CB	VAL	63	49.253	41.782	44.854	1.00	27.55
ATOM	621	CG1	VAL	63	49.949	41.351	43.592	1.00	25.68
ATOM	622	CG2	VAL	63	50.042	42.918	45.473	1.00	24.53
ATOM	623	C	VAL	63	46.983	41.081	43.886	1.00	35.52
ATOM	624	O	VAL	63	47.022	40.853	42.669	1.00	37.20
ATOM	625	N	ALA	64	46.171	40.335	44.662	1.00	37.43
ATOM	626	H	ALA	64	46.264	40.394	45.637	1.00	0.00

15/145

FIGURE 1 (CONT.)

ATOM	627	CA	ALA	64	45.242	39.338	44.082	1.00	37.26
ATOM	628	CB	ALA	64	44.284	38.795	45.135	1.00	37.48
ATOM	629	C	ALA	64	44.359	39.907	42.962	1.00	36.85
ATOM	630	O	ALA	64	44.159	39.339	41.882	1.00	35.68
ATOM	631	N	GLN	65	43.917	41.131	43.280	1.00	35.68
ATOM	632	H	GLN	65	44.228	41.501	44.132	1.00	0.00
ATOM	633	CA	GLN	65	43.084	41.953	42.426	1.00	33.82
ATOM	634	CB	GLN	65	42.387	42.998	43.320	1.00	31.98
ATOM	635	CG	GLN	65	41.413	42.339	44.271	1.00	32.72
ATOM	636	CD	GLN	65	41.089	43.076	45.562	1.00	36.64
ATOM	637	OE1	GLN	65	40.593	44.193	45.593	1.00	39.18
ATOM	638	NE2	GLN	65	41.327	42.544	46.749	1.00	37.45
ATOM	639	HE21	GLN	65	41.804	41.694	46.796	1.00	0.00
ATOM	640	HE22	GLN	65	40.981	43.069	47.492	1.00	0.00
ATOM	641	C	GLN	65	43.850	42.630	41.287	1.00	34.72
ATOM	642	O	GLN	65	43.338	43.597	40.716	1.00	39.31
ATOM	643	N	MET	66	45.030	42.187	40.841	1.00	33.73
ATOM	644	H	MET	66	45.401	41.357	41.212	1.00	0.00
ATOM	645	CA	MET	66	45.773	42.902	39.790	1.00	32.72
ATOM	646	CB	MET	66	47.164	43.337	40.337	1.00	30.79
ATOM	647	CG	MET	66	47.055	44.645	41.125	1.00	33.02
ATOM	648	SD	MET	66	48.593	45.437	41.680	1.00	30.39
ATOM	649	CE	MET	66	49.703	44.956	40.404	1.00	34.75
ATOM	650	C	MET	66	45.992	42.217	38.441	1.00	33.11
ATOM	651	O	MET	66	46.232	41.002	38.381	1.00	32.31
ATOM	652	N	SER	67	45.910	42.951	37.311	1.00	33.02
ATOM	653	H	SER	67	45.580	43.859	37.394	1.00	0.00
ATOM	654	CA	SER	67	46.184	42.362	35.973	1.00	34.10
ATOM	655	CB	SER	67	45.507	43.030	34.764	1.00	33.83
ATOM	656	OG	SER	67	44.178	43.505	34.864	1.00	37.19
ATOM	657	HG	SER	67	44.119	44.205	35.528	1.00	0.00
ATOM	658	C	SER	67	47.653	42.496	35.597	1.00	32.59
ATOM	659	O	SER	67	48.275	43.464	35.991	1.00	30.48
ATOM	660	N	VAL	68	48.316	41.628	34.838	1.00	34.29
ATOM	661	H	VAL	68	47.840	40.800	34.613	1.00	0.00
ATOM	662	CA	VAL	68	49.722	41.820	34.422	1.00	32.97
ATOM	663	CB	VAL	68	50.157	40.543	33.651	1.00	34.46
ATOM	664	CG1	VAL	68	51.591	40.603	33.168	1.00	35.72
ATOM	665	CG2	VAL	68	50.084	39.361	34.615	1.00	34.40
ATOM	666	C	VAL	68	49.952	43.104	33.603	1.00	31.72
ATOM	667	O	VAL	68	49.329	43.415	32.581	1.00	31.58
ATOM	668	N	GLY	69	50.873	43.873	34.175	1.00	29.96
ATOM	669	H	GLY	69	51.430	43.484	34.882	1.00	0.00
ATOM	670	CA	GLY	69	51.150	45.221	33.737	1.00	29.11
ATOM	671	C	GLY	69	50.294	46.253	34.477	1.00	30.32

16/145

FIGURE 1 (CONT.)

ATOM	672	O	GLY	69	50.373	47.467	34.256	1.00	31.12
ATOM	673	N	GLN	70	49.372	45.806	35.326	1.00	30.54
ATOM	674	H	GLN	70	49.253	44.849	35.388	1.00	0.00
ATOM	675	CA	GLN	70	48.557	46.721	36.102	1.00	31.29
ATOM	676	CB	GLN	70	47.329	46.059	36.732	1.00	32.00
ATOM	677	CG	GLN	70	46.186	47.013	37.104	1.00	33.97
ATOM	678	CD	GLN	70	44.926	46.303	37.579	1.00	36.12
ATOM	679	OE1	GLN	70	44.442	45.295	37.062	1.00	40.80
ATOM	680	NE2	GLN	70	44.305	46.714	38.648	1.00	37.28
ATOM	681	HE21	GLN	70	43.501	46.189	38.841	1.00	0.00
ATOM	682	HE22	GLN	70	44.665	47.431	39.193	1.00	0.00
ATOM	683	C	GLN	70	49.414	47.258	37.236	1.00	32.86
ATOM	684	O	GLN	70	50.041	46.527	38.012	1.00	31.95
ATOM	685	N	ARG	71	49.491	48.585	37.152	1.00	32.49
ATOM	686	H	ARG	71	49.202	48.957	36.292	1.00	0.00
ATOM	687	CA	ARG	71	50.099	49.470	38.132	1.00	31.24
ATOM	688	CB	ARG	71	50.891	50.555	37.374	1.00	33.82
ATOM	689	CG	ARG	71	51.417	51.583	38.328	1.00	40.25
ATOM	690	CD	ARG	71	52.293	52.658	37.744	1.00	46.99
ATOM	691	NE	ARG	71	51.645	53.546	36.778	1.00	50.72
ATOM	692	HE	ARG	71	50.723	53.375	36.497	1.00	0.00
ATOM	693	CZ	ARG	71	52.315	54.601	36.262	1.00	51.22
ATOM	694	NH1	ARG	71	51.719	55.352	35.326	1.00	48.94
ATOM	695	HH11	ARG	71	50.799	55.118	35.012	1.00	0.00
ATOM	696	HH12	ARG	71	52.204	56.132	34.928	1.00	0.00
ATOM	697	NH2	ARG	71	53.552	54.931	36.692	1.00	49.74
ATOM	698	HH21	ARG	71	53.996	54.400	37.413	1.00	0.00
ATOM	699	HH22	ARG	71	54.022	55.720	36.296	1.00	0.00
ATOM	700	C	ARG	71	48.963	50.061	38.970	1.00	28.83
ATOM	701	O	ARG	71	48.120	50.804	38.454	1.00	28.36
ATOM	702	N	ALA	72	48.888	49.750	40.256	1.00	27.78
ATOM	703	H	ALA	72	49.604	49.197	40.635	1.00	0.00
ATOM	704	CA	ALA	72	47.806	50.195	41.123	1.00	27.48
ATOM	705	CB	ALA	72	46.778	49.108	41.359	1.00	28.71
ATOM	706	C	ALA	72	48.226	50.619	42.507	1.00	27.52
ATOM	707	O	ALA	72	49.211	50.140	43.033	1.00	30.60
ATOM	708	N	LYS	73	47.444	51.491	43.110	1.00	27.01
ATOM	709	H	LYS	73	46.705	51.845	42.584	1.00	0.00
ATOM	710	CA	LYS	73	47.578	51.987	44.470	1.00	25.46
ATOM	711	CB	LYS	73	47.274	53.480	44.495	1.00	24.08
ATOM	712	CG	LYS	73	46.995	54.164	45.817	1.00	23.30
ATOM	713	CD	LYS	73	47.096	55.658	45.582	1.00	25.76
ATOM	714	CE	LYS	73	46.470	56.399	46.760	1.00	30.11
ATOM	715	NZ	LYS	73	46.525	57.846	46.563	1.00	33.42
ATOM	716	HZ1	LYS	73	45.930	58.104	45.750	1.00	0.00

17/145

FIGURE 1 (CONT.)

ATOM	717	HZ2	LYS	73	47.506	58.142	46.377	1.00	0.00
ATOM	718	HZ3	LYS	73	46.176	58.328	47.415	1.00	0.00
ATOM	719	C	LYS	73	46.673	51.282	45.465	1.00	26.41
ATOM	720	O	LYS	73	45.451	51.469	45.536	1.00	24.57
ATOM	721	N	LEU	74	47.354	50.437	46.231	1.00	28.26
ATOM	722	H	LEU	74	48.315	50.348	46.050	1.00	0.00
ATOM	723	CA	LEU	74	46.744	49.689	47.337	1.00	27.51
ATOM	724	CB	LEU	74	47.476	48.406	47.689	1.00	24.45
ATOM	725	CG	LEU	74	48.142	47.654	46.592	1.00	23.35
ATOM	726	CD1	LEU	74	48.902	46.472	47.145	1.00	25.32
ATOM	727	CD2	LEU	74	47.099	47.184	45.657	1.00	20.90
ATOM	728	C	LEU	74	46.826	50.539	48.591	1.00	28.08
ATOM	729	O	LEU	74	47.908	50.660	49.169	1.00	30.35
ATOM	730	N	THR	75	45.760	51.225	48.992	1.00	27.67
ATOM	731	H	THR	75	45.015	51.343	48.362	1.00	0.00
ATOM	732	CA	THR	75	45.749	51.891	50.286	1.00	25.75
ATOM	733	CB	THR	75	44.785	53.034	50.323	1.00	24.20
ATOM	734	OG1	THR	75	45.017	53.894	49.214	1.00	25.23
ATOM	735	HG1	THR	75	44.150	54.174	48.886	1.00	0.00
ATOM	736	CG2	THR	75	45.003	53.828	51.565	1.00	26.72
ATOM	737	C	THR	75	45.307	50.848	51.304	1.00	28.10
ATOM	738	O	THR	75	44.208	50.287	51.324	1.00	30.18
ATOM	739	N	ILE	76	46.261	50.457	52.125	1.00	29.77
ATOM	740	H	ILE	76	47.151	50.869	52.049	1.00	0.00
ATOM	741	CA	ILE	76	46.029	49.433	53.125	1.00	29.87
ATOM	742	CB	ILE	76	47.209	48.529	53.200	1.00	26.82
ATOM	743	CG2	ILE	76	46.897	47.388	54.152	1.00	23.97
ATOM	744	CG1	ILE	76	47.539	48.069	51.802	1.00	23.51
ATOM	745	CD1	ILE	76	48.881	47.377	51.662	1.00	25.59
ATOM	746	C	ILE	76	45.775	50.004	54.505	1.00	33.06
ATOM	747	O	ILE	76	46.367	50.991	54.937	1.00	34.29
ATOM	748	N	SER	77	44.836	49.364	55.187	1.00	34.85
ATOM	749	H	SER	77	44.324	48.700	54.684	1.00	0.00
ATOM	750	CA	SER	77	44.452	49.714	56.553	1.00	34.94
ATOM	751	CB	SER	77	42.973	49.458	56.706	1.00	32.22
ATOM	752	OG	SER	77	42.697	48.094	56.374	1.00	30.43
ATOM	753	HG	SER	77	43.342	47.549	56.862	1.00	0.00
ATOM	754	C	SER	77	45.198	48.960	57.668	1.00	36.01
ATOM	755	O	SER	77	45.059	47.728	57.699	1.00	35.63
ATOM	756	N	PRO	78	45.870	49.574	58.665	1.00	36.58
ATOM	757	CD	PRO	78	45.484	50.863	59.233	1.00	36.06
ATOM	758	CA	PRO	78	46.872	48.931	59.528	1.00	37.13
ATOM	759	CB	PRO	78	46.992	49.820	60.742	1.00	36.00
ATOM	760	CG	PRO	78	45.692	50.610	60.723	1.00	37.95
ATOM	761	C	PRO	78	46.633	47.494	59.941	1.00	37.64

18/145

FIGURE 1 (CONT.)

ATOM	762	O	PRO	78	47.578	46.732	60.008	1.00	38.53
ATOM	763	N	ASP	79	45.408	47.034	60.163	1.00	39.49
ATOM	764	H	ASP	79	44.663	47.656	60.065	1.00	0.00
ATOM	765	CA	ASP	79	45.177	45.645	60.564	1.00	41.87
ATOM	766	CB	ASP	79	43.712	45.491	60.999	1.00	43.28
ATOM	767	CG	ASP	79	42.701	45.788	59.902	1.00	42.93
ATOM	768	OD1	ASP	79	41.995	44.845	59.498	1.00	43.41
ATOM	769	OD2	ASP	79	42.655	46.944	59.469	1.00	38.42
ATOM	770	C	ASP	79	45.513	44.630	59.472	1.00	41.98
ATOM	771	O	ASP	79	45.844	43.466	59.696	1.00	44.22
ATOM	772	N	TYR	80	45.429	45.108	58.235	1.00	41.78
ATOM	773	H	TYR	80	45.037	45.983	58.138	1.00	0.00
ATOM	774	CA	TYR	80	45.856	44.334	57.068	1.00	40.72
ATOM	775	CB	TYR	80	44.710	44.529	55.976	1.00	40.86
ATOM	776	CG	TYR	80	43.773	43.307	55.929	1.00	42.68
ATOM	777	CD1	TYR	80	44.106	42.202	56.747	1.00	46.71
ATOM	778	CE1	TYR	80	43.461	40.963	56.672	1.00	45.23
ATOM	779	CD2	TYR	80	42.715	43.157	55.020	1.00	42.41
ATOM	780	CE2	TYR	80	42.056	41.899	54.939	1.00	44.31
ATOM	781	CZ	TYR	80	42.447	40.803	55.756	1.00	44.01
ATOM	782	OH	TYR	80	41.969	39.510	55.638	1.00	41.07
ATOM	783	HH	TYR	80	41.329	39.467	54.920	1.00	0.00
ATOM	784	C	TYR	80	47.294	44.681	56.595	1.00	39.44
ATOM	785	O	TYR	80	47.716	44.474	55.458	1.00	38.04
ATOM	786	N	ALA	81	48.055	45.151	57.604	1.00	37.51
ATOM	787	H	ALA	81	47.627	45.151	58.481	1.00	0.00
ATOM	788	CA	ALA	81	49.438	45.627	57.590	1.00	34.06
ATOM	789	CB	ALA	81	49.453	47.121	57.265	1.00	30.75
ATOM	790	C	ALA	81	50.075	45.394	58.987	1.00	33.78
ATOM	791	O	ALA	81	50.153	44.241	59.419	1.00	33.43
ATOM	792	N	TYR	82	50.478	46.396	59.797	1.00	32.85
ATOM	793	H	TYR	82	50.267	47.306	59.519	1.00	0.00
ATOM	794	CA	TYR	82	51.169	46.176	61.081	1.00	34.87
ATOM	795	CB	TYR	82	52.405	47.096	61.027	1.00	28.44
ATOM	796	CG	TYR	82	53.289	46.636	59.863	1.00	24.90
ATOM	797	CD1	TYR	82	53.328	47.357	58.674	1.00	25.10
ATOM	798	CE1	TYR	82	53.986	46.866	57.544	1.00	21.45
ATOM	799	CD2	TYR	82	53.948	45.409	59.913	1.00	24.80
ATOM	800	CE2	TYR	82	54.599	44.910	58.794	1.00	22.97
ATOM	801	CZ	TYR	82	54.609	45.645	57.621	1.00	21.85
ATOM	802	OH	TYR	82	55.259	45.136	56.533	1.00	24.65
ATOM	803	HH	TYR	82	55.256	45.782	55.814	1.00	0.00
ATOM	804	C	TYR	82	50.379	46.316	62.413	1.00	40.53
ATOM	805	O	TYR	82	50.766	45.858	63.501	1.00	42.10
ATOM	806	N	GLY	83	49.197	46.954	62.321	1.00	45.31

19/145

FIGURE 1 (CONT.)

ATOM	807	H	GLY	83	48.945	47.208	61.412	1.00	0.00
ATOM	808	CA	GLY	83	48.187	47.156	63.377	1.00	47.72
ATOM	809	C	GLY	83	48.507	47.941	64.651	1.00	50.23
ATOM	810	O	GLY	83	48.115	49.101	64.910	1.00	52.47
ATOM	811	N	ALA	84	49.195	47.183	65.493	1.00	49.36
ATOM	812	H	ALA	84	49.431	46.273	65.210	1.00	0.00
ATOM	813	CA	ALA	84	49.556	47.712	66.797	1.00	47.15
ATOM	814	CB	ALA	84	49.196	46.683	67.890	1.00	50.91
ATOM	815	C	ALA	84	51.029	48.053	66.918	1.00	43.75
ATOM	816	O	ALA	84	51.408	49.202	67.136	1.00	38.36
ATOM	817	N	THR	85	51.811	46.998	66.682	1.00	40.44
ATOM	818	H	THR	85	51.398	46.173	66.357	1.00	0.00
ATOM	819	CA	THR	85	53.258	47.031	66.838	1.00	40.70
ATOM	820	CB	THR	85	53.831	45.608	66.953	1.00	38.80
ATOM	821	OG1	THR	85	53.559	44.877	65.764	1.00	39.70
ATOM	822	HG1	THR	85	54.155	45.179	65.057	1.00	0.00
ATOM	823	CG2	THR	85	53.186	44.871	68.096	1.00	40.87
ATOM	824	C	THR	85	54.089	47.729	65.773	1.00	41.15
ATOM	825	O	THR	85	55.298	47.904	65.936	1.00	43.48
ATOM	826	N	GLY	86	53.468	48.113	64.652	1.00	40.17
ATOM	827	H	GLY	86	52.514	47.924	64.589	1.00	0.00
ATOM	828	CA	GLY	86	54.191	48.689	63.524	1.00	37.20
ATOM	829	C	GLY	86	55.336	47.771	63.059	1.00	35.37
ATOM	830	O	GLY	86	55.296	46.539	63.204	1.00	35.07
ATOM	831	N	HIS	87	56.406	48.357	62.517	1.00	33.89
ATOM	832	H	HIS	87	56.406	49.342	62.482	1.00	0.00
ATOM	833	CA	HIS	87	57.582	47.577	62.181	1.00	30.63
ATOM	834	CB	HIS	87	57.718	47.423	60.705	1.00	28.30
ATOM	835	CG	HIS	87	58.358	46.073	60.452	1.00	29.42
ATOM	836	CD2	HIS	87	59.654	45.893	60.034	1.00	27.09
ATOM	837	ND1	HIS	87	57.798	44.851	60.608	1.00	31.65
ATOM	838	HD1	HIS	87	56.875	44.656	60.899	1.00	0.00
ATOM	839	CE1	HIS	87	58.702	43.948	60.300	1.00	26.74
ATOM	840	NE2	HIS	87	59.798	44.597	59.962	1.00	26.86
ATOM	841	HE2	HIS	87	60.664	44.175	59.760	1.00	0.00
ATOM	842	C	HIS	87	58.797	48.303	62.709	1.00	30.65
ATOM	843	O	HIS	87	58.973	49.463	62.304	1.00	33.14
ATOM	844	N	PRO	88	59.629	47.719	63.592	1.00	31.15
ATOM	845	CD	PRO	88	59.379	46.404	64.186	1.00	29.92
ATOM	846	CA	PRO	88	60.857	48.346	64.178	1.00	30.23
ATOM	847	CB	PRO	88	61.619	47.176	64.798	1.00	32.28
ATOM	848	CG	PRO	88	60.512	46.225	65.232	1.00	32.35
ATOM	849	C	PRO	88	61.689	49.092	63.144	1.00	28.69
ATOM	850	O	PRO	88	62.099	48.464	62.172	1.00	30.18
ATOM	851	N	GLY	89	61.838	50.407	63.215	1.00	26.86

20/145

FIGURE 1 (CONT.)

ATOM	852	H	GLY	89	61.438	50.886	63.968	1.00	0.00
ATOM	853	CA	GLY	89	62.569	51.145	62.197	1.00	24.90
ATOM	854	C	GLY	89	61.784	51.826	61.062	1.00	28.34
ATOM	855	O	GLY	89	62.070	52.967	60.706	1.00	29.67
ATOM	856	N	ILE	90	60.765	51.249	60.426	1.00	28.41
ATOM	857	H	ILE	90	60.449	50.406	60.808	1.00	0.00
ATOM	858	CA	ILE	90	60.139	51.885	59.261	1.00	26.38
ATOM	859	CB	ILE	90	59.941	50.996	58.017	1.00	26.93
ATOM	860	CG2	ILE	90	60.961	51.343	56.962	1.00	28.43
ATOM	861	CG1	ILE	90	59.893	49.551	58.430	1.00	27.14
ATOM	862	CD1	ILE	90	61.188	48.805	58.717	1.00	30.53
ATOM	863	C	ILE	90	58.743	52.431	59.451	1.00	28.97
ATOM	864	O	ILE	90	58.472	53.597	59.139	1.00	31.50
ATOM	865	N	ILE	91	57.858	51.568	59.983	1.00	28.96
ATOM	866	H	ILE	91	58.227	50.776	60.415	1.00	0.00
ATOM	867	CA	ILE	91	56.408	51.819	60.100	1.00	27.73
ATOM	868	CB	ILE	91	55.616	50.558	59.655	1.00	26.34
ATOM	869	CG2	ILE	91	54.099	50.804	59.799	1.00	21.54
ATOM	870	CG1	ILE	91	56.016	50.183	58.232	1.00	22.37
ATOM	871	CD1	ILE	91	55.607	51.244	57.237	1.00	22.51
ATOM	872	C	ILE	91	55.936	52.198	61.507	1.00	29.11
ATOM	873	O	ILE	91	55.934	51.311	62.387	1.00	30.82
ATOM	874	N	PRO	92	55.529	53.451	61.774	1.00	28.57
ATOM	875	CD	PRO	92	55.492	54.537	60.803	1.00	28.83
ATOM	876	CA	PRO	92	54.980	53.862	63.063	1.00	31.00
ATOM	877	CB	PRO	92	54.698	55.328	62.808	1.00	30.11
ATOM	878	CG	PRO	92	54.379	55.401	61.332	1.00	29.05
ATOM	879	C	PRO	92	53.767	53.013	63.522	1.00	33.43
ATOM	880	O	PRO	92	53.078	52.465	62.653	1.00	35.46
ATOM	881	N	PRO	93	53.421	52.766	64.793	1.00	34.10
ATOM	882	CD	PRO	93	54.236	53.010	65.975	1.00	35.74
ATOM	883	CA	PRO	93	52.225	52.023	65.158	1.00	35.34
ATOM	884	CB	PRO	93	52.246	52.021	66.698	1.00	35.19
ATOM	885	CG	PRO	93	53.200	53.099	67.090	1.00	34.66
ATOM	886	C	PRO	93	50.921	52.554	64.557	1.00	36.07
ATOM	887	O	PRO	93	50.777	53.728	64.200	1.00	36.07
ATOM	888	N	HIS	94	49.951	51.664	64.364	1.00	38.60
ATOM	889	H	HIS	94	50.112	50.752	64.681	1.00	0.00
ATOM	890	CA	HIS	94	48.654	52.037	63.807	1.00	40.88
ATOM	891	CB	HIS	94	47.973	52.797	64.945	1.00	43.90
ATOM	892	CG	HIS	94	46.506	53.091	64.765	1.00	47.81
ATOM	893	CD2	HIS	94	45.980	54.366	64.651	1.00	50.92
ATOM	894	ND1	HIS	94	45.514	52.220	64.697	1.00	50.10
ATOM	895	HD1	HIS	94	45.559	51.268	64.927	1.00	0.00
ATOM	896	CE1	HIS	94	44.405	52.916	64.540	1.00	52.77

FIGURE 1 (CONT.)

ATOM	897	NE2	HIS	94	44.689	54.203	64.513	1.00	51.50
ATOM	898	HE2	HIS	94	44.047	54.925	64.360	1.00	0.00
ATOM	899	C	HIS	94	48.652	52.805	62.461	1.00	39.67
ATOM	900	O	HIS	94	47.983	53.828	62.267	1.00	39.97
ATOM	901	N	ALA	95	49.370	52.224	61.490	1.00	37.99
ATOM	902	H	ALA	95	49.906	51.451	61.740	1.00	0.00
ATOM	903	CA	ALA	95	49.546	52.796	60.144	1.00	35.23
ATOM	904	CB	ALA	95	51.037	52.985	59.887	1.00	35.82
ATOM	905	C	ALA	95	48.975	52.194	58.850	1.00	32.11
ATOM	906	O	ALA	95	49.143	51.039	58.480	1.00	32.00
ATOM	907	N	THR	96	48.259	53.094	58.214	1.00	30.85
ATOM	908	H	THR	96	48.116	53.929	58.707	1.00	0.00
ATOM	909	CA	THR	96	47.609	52.990	56.922	1.00	31.08
ATOM	910	CB	THR	96	46.473	54.017	56.729	1.00	33.73
ATOM	911	OG1	THR	96	45.609	53.994	57.882	1.00	35.36
ATOM	912	HG1	THR	96	45.030	54.760	57.848	1.00	0.00
ATOM	913	CG2	THR	96	45.728	53.738	55.425	1.00	32.78
ATOM	914	C	THR	96	48.677	53.368	55.918	1.00	31.50
ATOM	915	O	THR	96	49.117	54.515	55.833	1.00	32.50
ATOM	916	N	LEU	97	49.022	52.411	55.090	1.00	32.18
ATOM	917	H	LEU	97	48.454	51.611	55.101	1.00	0.00
ATOM	918	CA	LEU	97	50.135	52.449	54.142	1.00	30.94
ATOM	919	CB	LEU	97	50.987	51.207	54.306	1.00	31.46
ATOM	920	CG	LEU	97	51.258	50.762	55.748	1.00	33.64
ATOM	921	CD1	LEU	97	51.834	49.363	55.688	1.00	34.90
ATOM	922	CD2	LEU	97	52.152	51.778	56.484	1.00	32.11
ATOM	923	C	LEU	97	49.683	52.486	52.701	1.00	30.16
ATOM	924	O	LEU	97	49.034	51.522	52.293	1.00	31.15
ATOM	925	N	VAL	98	49.966	53.506	51.881	1.00	29.23
ATOM	926	H	VAL	98	50.622	54.176	52.168	1.00	0.00
ATOM	927	CA	VAL	98	49.521	53.445	50.494	1.00	25.96
ATOM	928	CB	VAL	98	49.020	54.858	49.919	1.00	24.00
ATOM	929	CG1	VAL	98	48.545	55.782	51.069	1.00	17.45
ATOM	930	CG2	VAL	98	50.080	55.498	49.064	1.00	25.60
ATOM	931	C	VAL	98	50.728	52.914	49.742	1.00	28.61
ATOM	932	O	VAL	98	51.906	53.252	49.955	1.00	28.41
ATOM	933	N	PHE	99	50.422	51.896	48.960	1.00	30.13
ATOM	934	H	PHE	99	49.520	51.533	49.008	1.00	0.00
ATOM	935	CA	PHE	99	51.431	51.242	48.145	1.00	28.95
ATOM	936	CB	PHE	99	51.504	49.755	48.424	1.00	27.30
ATOM	937	CG	PHE	99	52.302	49.292	49.623	1.00	28.31
ATOM	938	CD1	PHE	99	51.689	49.213	50.885	1.00	27.04
ATOM	939	CD2	PHE	99	53.631	48.894	49.439	1.00	26.44
ATOM	940	CE1	PHE	99	52.418	48.727	51.968	1.00	25.08
ATOM	941	CE2	PHE	99	54.342	48.413	50.531	1.00	25.08

22/145

FIGURE 1 (CONT.)

ATOM	942	CZ	PHE	99	53.738	48.329	51.789	1.00	25.86
ATOM	943	C	PHE	99	51.211	51.366	46.646	1.00	29.41
ATOM	944	O	PHE	99	50.248	50.784	46.111	1.00	28.62
ATOM	945	N	ASP	100	52.066	52.100	45.923	1.00	27.90
ATOM	946	H	ASP	100	52.790	52.603	46.356	1.00	0.00
ATOM	947	CA	ASP	100	51.933	51.986	44.484	1.00	27.65
ATOM	948	CB	ASP	100	52.515	53.213	43.786	1.00	29.75
ATOM	949	CG	ASP	100	52.444	52.983	42.290	1.00	33.48
ATOM	950	OD1	ASP	100	51.353	52.728	41.787	1.00	37.53
ATOM	951	OD2	ASP	100	53.481	52.982	41.620	1.00	38.98
ATOM	952	C	ASP	100	52.653	50.706	44.034	1.00	24.82
ATOM	953	O	ASP	100	53.860	50.593	44.178	1.00	25.12
ATOM	954	N	VAL	101	51.943	49.696	43.554	1.00	23.79
ATOM	955	H	VAL	101	50.973	49.812	43.528	1.00	0.00
ATOM	956	CA	VAL	101	52.489	48.409	43.126	1.00	23.21
ATOM	957	CB	VAL	101	51.826	47.263	43.990	1.00	21.54
ATOM	958	CG1	VAL	101	51.996	45.848	43.456	1.00	18.74
ATOM	959	CG2	VAL	101	52.550	47.246	45.312	1.00	17.06
ATOM	960	C	VAL	101	52.277	48.151	41.636	1.00	25.95
ATOM	961	O	VAL	101	51.190	48.341	41.120	1.00	29.28
ATOM	962	N	GLU	102	53.269	47.725	40.869	1.00	27.01
ATOM	963	H	GLU	102	54.162	47.669	41.268	1.00	0.00
ATOM	964	CA	GLU	102	53.092	47.385	39.474	1.00	28.99
ATOM	965	CB	GLU	102	54.066	48.215	38.645	1.00	33.82
ATOM	966	CG	GLU	102	54.184	47.980	37.124	1.00	37.96
ATOM	967	CD	GLU	102	55.526	48.447	36.530	1.00	43.93
ATOM	968	OE1	GLU	102	56.546	48.494	37.239	1.00	44.49
ATOM	969	OE2	GLU	102	55.566	48.761	35.335	1.00	46.19
ATOM	970	C	GLU	102	53.331	45.895	39.233	1.00	29.60
ATOM	971	O	GLU	102	54.370	45.374	39.647	1.00	30.02
ATOM	972	N	LEU	103	52.428	45.157	38.593	1.00	27.97
ATOM	973	H	LEU	103	51.593	45.582	38.324	1.00	0.00
ATOM	974	CA	LEU	103	52.674	43.754	38.315	1.00	28.42
ATOM	975	CB	LEU	103	51.353	42.980	38.146	1.00	27.72
ATOM	976	CG	LEU	103	51.090	41.665	38.900	1.00	29.71
ATOM	977	CD1	LEU	103	49.805	41.113	38.317	1.00	27.63
ATOM	978	CD2	LEU	103	52.216	40.615	38.756	1.00	27.20
ATOM	979	C	LEU	103	53.514	43.564	37.047	1.00	28.71
ATOM	980	O	LEU	103	53.080	43.813	35.922	1.00	32.25
ATOM	981	N	LEU	104	54.748	43.120	37.245	1.00	27.89
ATOM	982	H	LEU	104	55.012	42.922	38.169	1.00	0.00
ATOM	983	CA	LEU	104	55.689	42.876	36.179	1.00	25.74
ATOM	984	CB	LEU	104	57.131	42.886	36.683	1.00	23.34
ATOM	985	CG	LEU	104	57.710	43.912	37.645	1.00	23.01
ATOM	986	CD1	LEU	104	59.188	43.777	37.513	1.00	22.54

23/145

FIGURE 1 (CONT.)

ATOM	987	CD2	LEU	104	57.459	45.337	37.279	1.00	23.08
ATOM	988	C	LEU	104	55.484	41.535	35.492	1.00	27.74
ATOM	989	O	LEU	104	55.166	41.470	34.317	1.00	29.64
ATOM	990	N	LYS	105	55.637	40.425	36.204	1.00	28.91
ATOM	991	H	LYS	105	55.672	40.516	37.179	1.00	0.00
ATOM	992	CA	LYS	105	55.664	39.089	35.617	1.00	28.20
ATOM	993	CB	LYS	105	57.105	38.601	35.415	1.00	27.28
ATOM	994	CG	LYS	105	57.705	38.570	34.015	1.00	29.13
ATOM	995	CD	LYS	105	58.941	37.649	33.955	1.00	28.39
ATOM	996	CE	LYS	105	58.471	36.191	34.022	1.00	31.50
ATOM	997	NZ	LYS	105	59.563	35.242	34.103	1.00	31.35
ATOM	998	HZ1	LYS	105	59.180	34.287	34.251	1.00	0.00
ATOM	999	HZ2	LYS	105	60.183	35.494	34.899	1.00	0.00
ATOM	1000	HZ3	LYS	105	60.105	35.266	33.216	1.00	0.00
ATOM	1001	C	LYS	105	54.976	38.051	36.489	1.00	28.35
ATOM	1002	O	LYS	105	54.370	38.402	37.480	1.00	27.82
ATOM	1003	N	LEU	106	55.022	36.782	36.081	1.00	30.95
ATOM	1004	H	LEU	106	55.356	36.625	35.175	1.00	0.00
ATOM	1005	CA	LEU	106	54.616	35.586	36.844	1.00	35.17
ATOM	1006	CB	LEU	106	53.242	34.999	36.578	1.00	33.38
ATOM	1007	CG	LEU	106	51.952	35.717	36.750	1.00	33.64
ATOM	1008	CD1	LEU	106	51.859	36.455	38.091	1.00	30.30
ATOM	1009	CD2	LEU	106	51.841	36.587	35.514	1.00	37.34
ATOM	1010	C	LEU	106	55.521	34.414	36.450	1.00	36.29
ATOM	1011	O	LEU	106	56.067	34.339	35.344	1.00	37.48
ATOM	1012	N	GLU	107	55.707	33.475	37.344	1.00	37.84
ATOM	1013	H	GLU	107	55.235	33.508	38.201	1.00	0.00
ATOM	1014	CA	GLU	107	56.599	32.345	37.112	1.00	39.89
ATOM	1015	CB	GLU	107	58.043	32.822	37.214	1.00	40.97
ATOM	1016	CG	GLU	107	58.321	33.971	38.226	1.00	42.27
ATOM	1017	CD	GLU	107	59.781	34.393	38.327	1.00	43.06
ATOM	1018	OE1	GLU	107	60.436	33.959	39.285	1.00	44.20
ATOM	1019	OE2	GLU	107	60.245	35.133	37.449	1.00	40.58
ATOM	1020	C	GLU	107	56.339	31.243	38.131	1.00	41.09
ATOM	1021	O	GLU	107	55.419	31.432	38.956	1.00	45.17

CALCINEURIN SUBUNIT A COORDINATES

	Atom		Type	Residue #	X	Y	Z	OCC	B
ATOM	1022	CB	ALA	24	84.175	45.346	46.445	1.00	50.31
ATOM	1023	C	ALA	24	83.049	45.548	48.634	1.00	49.53
ATOM	1024	O	ALA	24	81.801	45.480	48.725	1.00	48.08
ATOM	1025	HT1	ALA	24	83.506	42.768	46.656	1.00	0.00
ATOM	1026	HT2	ALA	24	82.099	43.702	46.895	1.00	0.00

FIGURE 1 (CONT.)

ATOM	1027	N	ALA	24	82.997	43.379	47.325	1.00	50.14
ATOM	1028	HT3	ALA	24	82.743	42.842	48.181	1.00	0.00
ATOM	1029	CA	ALA	24	83.776	44.567	47.691	1.00	49.48
ATOM	1030	N	ALA	25	83.824	46.440	49.286	1.00	47.16
ATOM	1031	H	ALA	25	84.752	46.604	49.015	1.00	0.00
ATOM	1032	CA	ALA	25	83.263	47.330	50.312	1.00	46.17
ATOM	1033	CB	ALA	25	83.226	46.548	51.621	1.00	48.69
ATOM	1034	C	ALA	25	83.999	48.656	50.524	1.00	43.20
ATOM	1035	O	ALA	25	84.803	48.938	49.631	1.00	43.07
ATOM	1036	N	ALA	26	83.751	49.430	51.619	1.00	40.97
ATOM	1037	H	ALA	26	83.041	49.124	52.217	1.00	0.00
ATOM	1038	CA	ALA	26	84.374	50.759	51.934	1.00	38.77
ATOM	1039	CB	ALA	26	83.910	51.874	50.922	1.00	38.27
ATOM	1040	C	ALA	26	84.222	51.429	53.331	1.00	36.45
ATOM	1041	O	ALA	26	83.144	51.518	53.958	1.00	32.84
ATOM	1042	N	ALA	27	85.367	51.993	53.764	1.00	36.14
ATOM	1043	H	ALA	27	86.093	52.091	53.118	1.00	0.00
ATOM	1044	CA	ALA	27	85.493	52.548	55.113	1.00	35.20
ATOM	1045	CB	ALA	27	85.761	51.335	55.977	1.00	38.09
ATOM	1046	C	ALA	27	86.403	53.720	55.596	1.00	35.93
ATOM	1047	O	ALA	27	86.983	54.503	54.815	1.00	37.21
ATOM	1048	N	ALA	28	86.544	53.867	56.947	1.00	34.19
ATOM	1049	H	ALA	28	86.111	53.208	57.520	1.00	0.00
ATOM	1050	CA	ALA	28	87.237	54.988	57.578	1.00	31.95
ATOM	1051	CB	ALA	28	86.194	56.174	57.561	1.00	30.78
ATOM	1052	C	ALA	28	88.057	55.125	58.930	1.00	31.17
ATOM	1053	O	ALA	28	88.123	54.384	59.921	1.00	28.93
ATOM	1054	N	ALA	29	88.852	56.147	58.583	1.00	28.83
ATOM	1055	H	ALA	29	88.846	56.328	57.623	1.00	0.00
ATOM	1056	CA	ALA	29	89.774	57.001	59.262	1.00	23.93
ATOM	1057	CB	ALA	29	91.116	57.198	58.530	1.00	22.54
ATOM	1058	C	ALA	29	89.037	58.317	59.041	1.00	22.19
ATOM	1059	O	ALA	29	88.652	58.615	57.908	1.00	21.75
ATOM	1060	N	ALA	30	88.737	59.091	60.058	1.00	21.20
ATOM	1061	H	ALA	30	88.935	58.783	60.964	1.00	0.00
ATOM	1062	CA	ALA	30	88.135	60.389	59.851	1.00	22.28
ATOM	1063	CB	ALA	30	87.373	60.772	61.135	1.00	19.34
ATOM	1064	C	ALA	30	89.174	61.469	59.479	1.00	21.66
ATOM	1065	O	ALA	30	90.193	61.684	60.152	1.00	20.96
ATOM	1066	N	ALA	31	88.961	62.168	58.374	1.00	20.60
ATOM	1067	H	ALA	31	88.121	61.993	57.904	1.00	0.00
ATOM	1068	CA	ALA	31	89.856	63.258	57.981	1.00	20.34
ATOM	1069	CB	ALA	31	89.352	63.883	56.667	1.00	19.97
ATOM	1070	C	ALA	31	89.960	64.354	59.065	1.00	22.46
ATOM	1071	O	ALA	31	88.958	64.783	59.650	1.00	22.75

25/145

FIGURE 1 (CONT.)

ATOM	1072	N	ALA	32	91.213	64.693	59.406	1.00	22.27
ATOM	1073	H	ALA	32	91.890	64.113	59.010	1.00	0.00
ATOM	1074	CA	ALA	32	91.670	65.720	60.377	1.00	21.07
ATOM	1075	CB	ALA	32	93.101	65.388	60.808	1.00	16.27
ATOM	1076	C	ALA	32	91.687	67.140	59.809	1.00	21.01
ATOM	1077	O	ALA	32	91.244	67.271	58.666	1.00	25.29
ATOM	1078	N	ALA	33	92.131	68.275	60.388	1.00	19.49
ATOM	1079	H	ALA	33	92.413	68.248	61.330	1.00	0.00
ATOM	1080	CA	ALA	33	92.349	69.492	59.581	1.00	16.51
ATOM	1081	CB	ALA	33	92.365	70.585	60.570	1.00	14.14
ATOM	1082	C	ALA	33	93.659	69.407	58.724	1.00	20.57
ATOM	1083	O	ALA	33	94.760	69.875	58.983	1.00	21.29
ATOM	1084	N	ALA	34	93.495	68.469	57.761	1.00	25.97
ATOM	1085	H	ALA	34	92.676	67.993	57.896	1.00	0.00
ATOM	1086	CA	ALA	34	94.225	67.896	56.585	1.00	21.13
ATOM	1087	CB	ALA	34	94.337	66.372	56.553	1.00	20.20
ATOM	1088	C	ALA	34	93.277	68.129	55.374	1.00	22.53
ATOM	1089	O	ALA	34	93.573	67.809	54.221	1.00	20.37
ATOM	1090	N	ALA	35	92.008	68.505	55.703	1.00	21.03
ATOM	1091	H	ALA	35	91.689	68.264	56.596	1.00	0.00
ATOM	1092	CA	ALA	35	91.063	69.017	54.731	1.00	18.49
ATOM	1093	CB	ALA	35	89.642	68.919	55.232	1.00	12.08
ATOM	1094	C	ALA	35	91.405	70.485	54.559	1.00	19.12
ATOM	1095	O	ALA	35	91.393	70.975	53.451	1.00	21.45
ATOM	1096	N	ASP	36	91.749	71.272	55.574	1.00	21.28
ATOM	1097	H	ASP	36	91.824	70.881	56.463	1.00	0.00
ATOM	1098	CA	ASP	36	91.997	72.703	55.380	1.00	24.10
ATOM	1099	CB	ASP	36	91.440	73.596	56.538	1.00	21.58
ATOM	1100	CG	ASP	36	89.912	73.763	56.542	1.00	29.14
ATOM	1101	OD1	ASP	36	89.223	72.967	57.218	1.00	32.83
ATOM	1102	OD2	ASP	36	89.398	74.679	55.881	1.00	24.50
ATOM	1103	C	ASP	36	93.474	72.946	55.291	1.00	27.46
ATOM	1104	O	ASP	36	94.204	72.675	56.231	1.00	30.17
ATOM	1105	N	ASN	37	94.039	73.366	54.193	1.00	31.18
ATOM	1106	H	ASN	37	93.499	73.442	53.376	1.00	0.00
ATOM	1107	CA	ASN	37	95.450	73.691	54.202	1.00	35.64
ATOM	1108	CB	ASN	37	96.184	72.664	53.350	1.00	40.99
ATOM	1109	CG	ASN	37	96.431	71.306	54.057	1.00	45.60
ATOM	1110	OD1	ASN	37	96.734	70.305	53.428	1.00	43.54
ATOM	1111	ND2	ASN	37	96.345	71.049	55.354	1.00	49.10
ATOM	1112	HD21	ASN	37	96.016	71.721	55.981	1.00	0.00
ATOM	1113	HD22	ASN	37	96.632	70.143	55.576	1.00	0.00
ATOM	1114	C	ASN	37	95.738	75.122	53.752	1.00	37.92
ATOM	1115	O	ASN	37	95.672	75.514	52.566	1.00	35.92
ATOM	1116	N	ASP	38	95.901	75.830	54.903	1.00	37.29

26/145

FIGURE 1 (CONT.)

ATOM	1117	H	ASP	38	95.865	75.291	55.717	1.00	0.00
ATOM	1118	CA	ASP	38	96.180	77.278	55.073	1.00	38.07
ATOM	1119	CB	ASP	38	97.561	77.498	54.509	1.00	40.31
ATOM	1120	CG	ASP	38	98.541	77.179	55.609	1.00	42.81
ATOM	1121	OD1	ASP	38	98.514	77.971	56.566	1.00	45.63
ATOM	1122	OD2	ASP	38	99.282	76.179	55.509	1.00	42.77
ATOM	1123	C	ASP	38	95.245	78.437	54.637	1.00	36.72
ATOM	1124	O	ASP	38	95.488	79.528	54.093	1.00	33.25
ATOM	1125	N	GLY	39	94.109	78.096	55.211	1.00	33.60
ATOM	1126	H	GLY	39	94.089	77.333	55.821	1.00	0.00
ATOM	1127	CA	GLY	39	92.908	78.825	55.000	1.00	32.50
ATOM	1128	C	GLY	39	91.939	77.938	54.218	1.00	31.26
ATOM	1129	O	GLY	39	90.868	77.557	54.671	1.00	32.03
ATOM	1130	N	LYS	40	92.432	77.520	53.067	1.00	28.47
ATOM	1131	H	LYS	40	93.384	77.673	52.895	1.00	0.00
ATOM	1132	CA	LYS	40	91.641	76.900	52.026	1.00	25.84
ATOM	1133	CB	LYS	40	92.323	77.223	50.677	1.00	30.80
ATOM	1134	CG	LYS	40	92.335	78.723	50.414	1.00	34.55
ATOM	1135	CD	LYS	40	92.946	79.268	49.119	1.00	37.54
ATOM	1136	CE	LYS	40	92.708	80.799	49.207	1.00	37.03
ATOM	1137	NZ	LYS	40	92.761	81.447	47.916	1.00	36.90
ATOM	1138	HZ1	LYS	40	93.684	81.256	47.478	1.00	0.00
ATOM	1139	HZ2	LYS	40	92.636	82.474	48.035	1.00	0.00
ATOM	1140	HZ3	LYS	40	92.003	81.076	47.308	1.00	0.00
ATOM	1141	C	LYS	40	91.353	75.423	52.119	1.00	22.41
ATOM	1142	O	LYS	40	92.213	74.623	52.481	1.00	19.83
ATOM	1143	N	PRO	41	90.123	75.002	51.861	1.00	22.00
ATOM	1144	CD	PRO	41	88.926	75.859	51.854	1.00	19.73
ATOM	1145	CA	PRO	41	89.793	73.581	51.904	1.00	20.61
ATOM	1146	CB	PRO	41	88.280	73.591	52.007	1.00	23.55
ATOM	1147	CG	PRO	41	87.929	74.975	52.564	1.00	21.04
ATOM	1148	C	PRO	41	90.364	72.866	50.704	1.00	20.28
ATOM	1149	O	PRO	41	90.512	73.429	49.616	1.00	21.97
ATOM	1150	N	ARG	42	90.801	71.625	50.873	1.00	21.79
ATOM	1151	H	ARG	42	90.765	71.246	51.768	1.00	0.00
ATOM	1152	CA	ARG	42	91.398	70.848	49.779	1.00	21.51
ATOM	1153	CB	ARG	42	92.578	69.977	50.301	1.00	20.84
ATOM	1154	CG	ARG	42	93.682	70.713	51.061	1.00	23.19
ATOM	1155	CD	ARG	42	94.970	69.950	51.308	1.00	26.44
ATOM	1156	NE	ARG	42	95.806	70.089	50.136	1.00	35.33
ATOM	1157	HE	ARG	42	95.464	69.665	49.322	1.00	0.00
ATOM	1158	CZ	ARG	42	97.001	70.731	50.007	1.00	40.01
ATOM	1159	NH1	ARG	42	97.498	70.823	48.761	1.00	41.01
ATOM	1160	HH11	ARG	42	96.993	70.432	47.990	1.00	0.00
ATOM	1161	HH12	ARG	42	98.371	71.286	48.603	1.00	0.00

27/145

FIGURE 1 (CONT.)

ATOM	1162	NH2	ARG	42	97.756	71.227	51.010	1.00	37.84
ATOM	1163	HH21	ARG	42	97.445	71.136	51.949	1.00	0.00
ATOM	1164	HH22	ARG	42	98.621	71.688	50.806	1.00	0.00
ATOM	1165	C	ARG	42	90.270	69.979	49.240	1.00	21.01
ATOM	1166	O	ARG	42	90.199	68.772	49.507	1.00	20.20
ATOM	1167	N	VAL	43	89.354	70.611	48.466	1.00	19.35
ATOM	1168	H	VAL	43	89.519	71.557	48.259	1.00	0.00
ATOM	1169	CA	VAL	43	88.113	69.934	48.037	1.00	17.98
ATOM	1170	CB	VAL	43	87.211	70.888	47.239	1.00	16.82
ATOM	1171	CG1	VAL	43	86.790	72.072	48.100	1.00	9.06
ATOM	1172	CG2	VAL	43	87.967	71.399	46.047	1.00	15.82
ATOM	1173	C	VAL	43	88.295	68.645	47.251	1.00	19.52
ATOM	1174	O	VAL	43	87.458	67.765	47.322	1.00	21.60
ATOM	1175	N	ASP	44	89.413	68.437	46.565	1.00	21.12
ATOM	1176	H	ASP	44	89.968	69.219	46.391	1.00	0.00
ATOM	1177	CA	ASP	44	89.822	67.148	46.006	1.00	21.78
ATOM	1178	CB	ASP	44	91.124	67.383	45.206	1.00	28.20
ATOM	1179	CG	ASP	44	92.394	67.906	45.944	1.00	35.44
ATOM	1180	OD1	ASP	44	92.327	68.730	46.878	1.00	35.94
ATOM	1181	OD2	ASP	44	93.489	67.474	45.559	1.00	39.50
ATOM	1182	C	ASP	44	90.011	66.084	47.106	1.00	20.71
ATOM	1183	O	ASP	44	89.446	64.998	47.028	1.00	21.62
ATOM	1184	N	ILE	45	90.691	66.359	48.234	1.00	21.23
ATOM	1185	H	ILE	45	91.069	67.256	48.333	1.00	0.00
ATOM	1186	CA	ILE	45	90.837	65.385	49.344	1.00	20.46
ATOM	1187	CB	ILE	45	91.637	66.032	50.521	1.00	17.75
ATOM	1188	CG2	ILE	45	91.674	65.154	51.789	1.00	10.96
ATOM	1189	CG1	ILE	45	93.043	66.299	49.992	1.00	17.65
ATOM	1190	CD1	ILE	45	93.781	65.018	49.525	1.00	19.86
ATOM	1191	C	ILE	45	89.500	64.868	49.879	1.00	22.50
ATOM	1192	O	ILE	45	89.252	63.664	50.079	1.00	25.21
ATOM	1193	N	LEU	46	88.674	65.900	50.097	1.00	21.62
ATOM	1194	H	LEU	46	89.068	66.785	49.955	1.00	0.00
ATOM	1195	CA	LEU	46	87.283	65.821	50.520	1.00	20.02
ATOM	1196	CB	LEU	46	86.814	67.258	50.794	1.00	18.61
ATOM	1197	CG	LEU	46	85.669	67.549	51.755	1.00	19.28
ATOM	1198	CD1	LEU	46	86.153	67.416	53.190	1.00	16.09
ATOM	1199	CD2	LEU	46	85.147	68.945	51.502	1.00	14.88
ATOM	1200	C	LEU	46	86.377	65.114	49.492	1.00	20.87
ATOM	1201	O	LEU	46	85.737	64.147	49.904	1.00	24.45
ATOM	1202	N	LYS	47	86.287	65.425	48.190	1.00	18.62
ATOM	1203	H	LYS	47	86.795	66.192	47.888	1.00	0.00
ATOM	1204	CA	LYS	47	85.448	64.708	47.224	1.00	17.99
ATOM	1205	CB	LYS	47	85.711	65.121	45.779	1.00	19.77
ATOM	1206	CG	LYS	47	84.841	64.479	44.680	1.00	18.97

28/145

FIGURE 1 (CONT.)

ATOM	1207	CD	LYS	47	85.448	64.900	43.349	1.00	20.85
ATOM	1208	CE	LYS	47	84.708	64.428	42.109	1.00	22.34
ATOM	1209	NZ	LYS	47	84.686	62.976	42.045	1.00	26.53
ATOM	1210	HZ1	LYS	47	84.238	62.670	41.157	1.00	0.00
ATOM	1211	HZ2	LYS	47	84.136	62.618	42.853	1.00	0.00
ATOM	1212	HZ3	LYS	47	85.658	62.608	42.097	1.00	0.00
ATOM	1213	C	LYS	47	85.708	63.234	47.258	1.00	17.49
ATOM	1214	O	LYS	47	84.814	62.412	47.436	1.00	20.23
ATOM	1215	N	ALA	48	86.986	62.898	47.182	1.00	17.49
ATOM	1216	H	ALA	48	87.658	63.615	47.118	1.00	0.00
ATOM	1217	CA	ALA	48	87.388	61.501	47.122	1.00	15.01
ATOM	1218	CB	ALA	48	88.817	61.460	46.795	1.00	12.93
ATOM	1219	C	ALA	48	87.166	60.656	48.356	1.00	15.68
ATOM	1220	O	ALA	48	86.875	59.466	48.294	1.00	19.82
ATOM	1221	N	HIS	49	87.337	61.267	49.525	1.00	16.17
ATOM	1222	H	HIS	49	87.713	62.175	49.481	1.00	0.00
ATOM	1223	CA	HIS	49	87.067	60.632	50.831	1.00	15.92
ATOM	1224	CB	HIS	49	87.526	61.488	52.023	1.00	16.45
ATOM	1225	CG	HIS	49	87.730	60.679	53.296	1.00	15.80
ATOM	1226	CD2	HIS	49	88.480	59.519	53.333	1.00	13.49
ATOM	1227	ND1	HIS	49	87.210	60.878	54.507	1.00	14.45
ATOM	1228	HD1	HIS	49	86.663	61.625	54.832	1.00	0.00
ATOM	1229	CE1	HIS	49	87.597	59.883	55.250	1.00	13.40
ATOM	1230	NE2	HIS	49	88.349	59.081	54.546	1.00	12.56
ATOM	1231	HE2	HIS	49	88.745	58.254	54.895	1.00	0.00
ATOM	1232	C	HIS	49	85.574	60.422	51.048	1.00	15.41
ATOM	1233	O	HIS	49	85.171	59.358	51.494	1.00	15.46
ATOM	1234	N	LEU	50	84.766	61.446	50.764	1.00	13.37
ATOM	1235	H	LEU	50	85.161	62.287	50.438	1.00	0.00
ATOM	1236	CA	LEU	50	83.323	61.347	50.836	1.00	13.25
ATOM	1237	CB	LEU	50	82.782	62.733	50.536	1.00	13.30
ATOM	1238	CG	LEU	50	83.158	63.821	51.521	1.00	14.86
ATOM	1239	CD1	LEU	50	82.473	65.084	51.124	1.00	15.86
ATOM	1240	CD2	LEU	50	82.678	63.496	52.928	1.00	18.66
ATOM	1241	C	LEU	50	82.780	60.271	49.884	1.00	13.94
ATOM	1242	O	LEU	50	82.019	59.406	50.317	1.00	14.16
ATOM	1243	N	MET	51	83.239	60.159	48.630	1.00	14.34
ATOM	1244	H	MET	51	83.854	60.847	48.296	1.00	0.00
ATOM	1245	CA	MET	51	82.741	59.112	47.734	1.00	15.28
ATOM	1246	CB	MET	51	83.320	59.254	46.318	1.00	16.58
ATOM	1247	CG	MET	51	82.625	60.245	45.394	1.00	17.87
ATOM	1248	SD	MET	51	83.380	60.334	43.748	1.00	26.04
ATOM	1249	CE	MET	51	82.325	59.123	43.021	1.00	15.44
ATOM	1250	C	MET	51	83.006	57.683	48.187	1.00	16.78
ATOM	1251	O	MET	51	82.349	56.713	47.782	1.00	20.27

29/145

FIGURE 1 (CONT.)

ATOM	1252	N	LYS	52	83.989	57.498	49.059	1.00	18.56
ATOM	1253	H	LYS	52	84.567	58.250	49.291	1.00	0.00
ATOM	1254	CA	LYS	52	84.259	56.168	49.608	1.00	18.69
ATOM	1255	CB	LYS	52	85.758	56.063	49.944	1.00	21.08
ATOM	1256	CG	LYS	52	86.754	56.437	48.817	1.00	20.81
ATOM	1257	CD	LYS	52	88.145	55.963	49.204	1.00	23.37
ATOM	1258	CE	LYS	52	89.286	56.611	48.391	1.00	30.03
ATOM	1259	NZ	LYS	52	89.767	57.894	48.945	1.00	31.58
ATOM	1260	HZ1	LYS	52	90.162	57.740	49.895	1.00	0.00
ATOM	1261	HZ2	LYS	52	88.976	58.568	48.999	1.00	0.00
ATOM	1262	HZ3	LYS	52	90.505	58.273	48.320	1.00	0.00
ATOM	1263	C	LYS	52	83.392	55.950	50.859	1.00	20.01
ATOM	1264	O	LYS	52	83.512	54.951	51.549	1.00	19.77
ATOM	1265	N	GLU	53	82.422	56.858	51.127	1.00	20.59
ATOM	1266	H	GLU	53	82.217	57.503	50.430	1.00	0.00
ATOM	1267	CA	GLU	53	81.601	56.903	52.322	1.00	19.86
ATOM	1268	CB	GLU	53	80.708	55.661	52.470	1.00	19.53
ATOM	1269	CG	GLU	53	79.683	55.436	51.403	1.00	17.55
ATOM	1270	CD	GLU	53	78.605	54.451	51.821	1.00	21.15
ATOM	1271	OE1	GLU	53	77.552	54.898	52.272	1.00	22.75
ATOM	1272	OE2	GLU	53	78.787	53.241	51.666	1.00	21.64
ATOM	1273	C	GLU	53	82.473	57.026	53.572	1.00	20.93
ATOM	1274	O	GLU	53	82.272	56.456	54.646	1.00	23.12
ATOM	1275	N	GLY	54	83.493	57.861	53.409	1.00	21.41
ATOM	1276	H	GLY	54	83.624	58.248	52.518	1.00	0.00
ATOM	1277	CA	GLY	54	84.414	58.189	54.467	1.00	17.93
ATOM	1278	C	GLY	54	83.902	59.384	55.263	1.00	19.98
ATOM	1279	O	GLY	54	83.184	60.289	54.791	1.00	16.56
ATOM	1280	N	ARG	55	84.290	59.363	56.539	1.00	20.47
ATOM	1281	H	ARG	55	84.651	58.538	56.911	1.00	0.00
ATOM	1282	CA	ARG	55	83.904	60.469	57.380	1.00	20.06
ATOM	1283	CB	ARG	55	83.234	59.873	58.603	1.00	22.16
ATOM	1284	CG	ARG	55	81.747	60.194	58.663	1.00	23.41
ATOM	1285	CD	ARG	55	81.109	59.524	59.839	1.00	25.27
ATOM	1286	NE	ARG	55	81.235	58.091	59.705	1.00	28.71
ATOM	1287	HE	ARG	55	81.595	57.717	58.874	1.00	0.00
ATOM	1288	CZ	ARG	55	80.864	57.233	60.672	1.00	33.66
ATOM	1289	NH1	ARG	55	81.053	55.913	60.461	1.00	34.62
ATOM	1290	HH11	ARG	55	81.455	55.597	59.602	1.00	0.00
ATOM	1291	HH12	ARG	55	80.781	55.251	61.160	1.00	0.00
ATOM	1292	NH2	ARG	55	80.310	57.645	61.833	1.00	31.92
ATOM	1293	HH21	ARG	55	80.186	58.617	62.012	1.00	0.00
ATOM	1294	HH22	ARG	55	80.044	56.969	62.520	1.00	0.00
ATOM	1295	C	ARG	55	84.971	61.486	57.786	1.00	21.37
ATOM	1296	O	ARG	55	86.184	61.265	57.626	1.00	21.45

30/145

FIGURE 1 (CONT.)

ATOM	1297	N	LEU	56	84.513	62.675	58.174	1.00	19.72
ATOM	1298	H	LEU	56	83.550	62.852	58.128	1.00	0.00
ATOM	1299	CA	LEU	56	85.407	63.670	58.705	1.00	20.97
ATOM	1300	CB	LEU	56	84.932	65.036	58.355	1.00	20.35
ATOM	1301	CG	LEU	56	85.412	65.653	57.071	1.00	20.05
ATOM	1302	CD1	LEU	56	85.363	64.655	55.919	1.00	24.78
ATOM	1303	CD2	LEU	56	84.515	66.833	56.775	1.00	20.80
ATOM	1304	C	LEU	56	85.518	63.574	60.204	1.00	21.58
ATOM	1305	O	LEU	56	84.787	62.817	60.842	1.00	21.68
ATOM	1306	N	GLU	57	86.478	64.249	60.811	1.00	23.10
ATOM	1307	H	GLU	57	87.164	64.703	60.282	1.00	0.00
ATOM	1308	CA	GLU	57	86.518	64.252	62.258	1.00	22.49
ATOM	1309	CB	GLU	57	87.942	64.672	62.604	1.00	21.78
ATOM	1310	CG	GLU	57	88.522	64.140	63.909	1.00	26.48
ATOM	1311	CD	GLU	57	88.742	62.624	64.078	1.00	31.32
ATOM	1312	OE1	GLU	57	87.880	61.995	64.703	1.00	33.93
ATOM	1313	OE2	GLU	57	89.770	62.070	63.640	1.00	29.95
ATOM	1314	C	GLU	57	85.387	65.216	62.675	1.00	22.20
ATOM	1315	O	GLU	57	85.268	66.287	62.059	1.00	25.00
ATOM	1316	N	GLU	58	84.464	64.910	63.603	1.00	21.96
ATOM	1317	H	GLU	58	84.481	64.003	63.973	1.00	0.00
ATOM	1318	CA	GLU	58	83.372	65.823	63.976	1.00	23.99
ATOM	1319	CB	GLU	58	82.860	65.433	65.384	1.00	25.99
ATOM	1320	CG	GLU	58	81.990	66.526	66.056	1.00	28.21
ATOM	1321	CD	GLU	58	80.680	66.059	66.652	1.00	30.88
ATOM	1322	OE1	GLU	58	79.740	65.727	65.915	1.00	30.11
ATOM	1323	OE2	GLU	58	80.615	66.045	67.874	1.00	32.71
ATOM	1324	C	GLU	58	83.642	67.348	63.952	1.00	22.49
ATOM	1325	O	GLU	58	82.883	68.194	63.491	1.00	23.84
ATOM	1326	N	THR	59	84.787	67.723	64.474	1.00	20.98
ATOM	1327	H	THR	59	85.363	67.037	64.870	1.00	0.00
ATOM	1328	CA	THR	59	85.198	69.118	64.558	1.00	18.39
ATOM	1329	CB	THR	59	86.334	69.142	65.624	1.00	14.67
ATOM	1330	OG1	THR	59	86.920	67.842	65.836	1.00	16.86
ATOM	1331	HG1	THR	59	87.274	67.850	66.735	1.00	0.00
ATOM	1332	CG2	THR	59	85.717	69.534	66.935	1.00	14.19
ATOM	1333	C	THR	59	85.564	69.758	63.222	1.00	16.68
ATOM	1334	O	THR	59	85.376	70.948	62.991	1.00	16.77
ATOM	1335	N	VAL	60	85.960	68.970	62.228	1.00	18.25
ATOM	1336	H	VAL	60	86.040	68.015	62.417	1.00	0.00
ATOM	1337	CA	VAL	60	86.306	69.495	60.898	1.00	18.64
ATOM	1338	CB	VAL	60	87.236	68.490	60.159	1.00	18.71
ATOM	1339	CG1	VAL	60	87.773	69.141	58.907	1.00	17.41
ATOM	1340	CG2	VAL	60	88.464	68.135	60.976	1.00	17.97
ATOM	1341	C	VAL	60	84.992	69.711	60.122	1.00	18.99

31/145

FIGURE 1 (CONT.)

ATOM	1342	O	VAL	60	84.756	70.714	59.437	1.00	19.51
ATOM	1343	N	ALA	61	84.084	68.744	60.283	1.00	16.96
ATOM	1344	H	ALA	61	84.367	67.954	60.788	1.00	0.00
ATOM	1345	CA	ALA	61	82.737	68.817	59.744	1.00	16.08
ATOM	1346	CB	ALA	61	82.007	67.552	60.235	1.00	11.73
ATOM	1347	C	ALA	61	82.092	70.125	60.248	1.00	17.37
ATOM	1348	O	ALA	61	81.720	71.003	59.472	1.00	19.75
ATOM	1349	N	LEU	62	82.059	70.374	61.564	1.00	19.84
ATOM	1350	H	LEU	62	82.355	69.654	62.163	1.00	0.00
ATOM	1351	CA	LEU	62	81.600	71.624	62.169	1.00	19.10
ATOM	1352	CB	LEU	62	81.736	71.523	63.667	1.00	20.23
ATOM	1353	CG	LEU	62	80.761	70.693	64.460	1.00	20.88
ATOM	1354	CD1	LEU	62	81.226	70.619	65.904	1.00	20.57
ATOM	1355	CD2	LEU	62	79.378	71.318	64.378	1.00	18.85
ATOM	1356	C	LEU	62	82.337	72.881	61.714	1.00	20.71
ATOM	1357	O	LEU	62	81.727	73.947	61.641	1.00	21.62
ATOM	1358	N	ARG	63	83.659	72.827	61.479	1.00	22.06
ATOM	1359	H	ARG	63	84.148	72.053	61.829	1.00	0.00
ATOM	1360	CA	ARG	63	84.416	73.939	60.895	1.00	20.95
ATOM	1361	CB	ARG	63	85.907	73.583	60.909	1.00	19.41
ATOM	1362	CG	ARG	63	86.817	74.726	60.475	1.00	18.04
ATOM	1363	CD	ARG	63	88.290	74.445	60.650	1.00	18.68
ATOM	1364	NE	ARG	63	89.030	75.361	59.784	1.00	23.34
ATOM	1365	HE	ARG	63	88.516	75.959	59.216	1.00	0.00
ATOM	1366	CZ	ARG	63	90.369	75.342	59.563	1.00	25.33
ATOM	1367	NH1	ARG	63	90.904	76.237	58.715	1.00	21.46
ATOM	1368	HH11	ARG	63	90.319	76.910	58.262	1.00	0.00
ATOM	1369	HH12	ARG	63	91.891	76.235	58.550	1.00	0.00
ATOM	1370	NH2	ARG	63	91.184	74.406	60.110	1.00	29.46
ATOM	1371	HH21	ARG	63	90.795	73.692	60.692	1.00	0.00
ATOM	1372	HH22	ARG	63	92.166	74.423	59.921	1.00	0.00
ATOM	1373	C	ARG	63	83.960	74.241	59.450	1.00	23.81
ATOM	1374	O	ARG	63	83.796	75.411	59.078	1.00	25.11
ATOM	1375	N	ILE	64	83.723	73.227	58.574	1.00	24.54
ATOM	1376	H	ILE	64	83.917	72.320	58.892	1.00	0.00
ATOM	1377	CA	ILE	64	83.218	73.436	57.193	1.00	22.65
ATOM	1378	CB	ILE	64	83.078	72.082	56.435	1.00	23.45
ATOM	1379	CG2	ILE	64	82.417	72.295	55.080	1.00	23.81
ATOM	1380	CG1	ILE	64	84.442	71.450	56.219	1.00	21.98
ATOM	1381	CD1	ILE	64	84.372	70.078	55.522	1.00	21.05
ATOM	1382	C	ILE	64	81.852	74.091	57.301	1.00	20.24
ATOM	1383	O	ILE	64	81.587	75.111	56.663	1.00	20.59
ATOM	1384	N	ILE	65	81.024	73.583	58.226	1.00	19.00
ATOM	1385	H	ILE	65	81.308	72.778	58.712	1.00	0.00
ATOM	1386	CA	ILE	65	79.691	74.171	58.441	1.00	20.73

32/145

FIGURE 1 (CONT.)

ATOM	1387	CB	ILE	65	78.859	73.225	59.345	1.00	17.60
ATOM	1388	CG2	ILE	65	77.529	73.853	59.547	1.00	18.37
ATOM	1389	CG1	ILE	65	78.564	71.874	58.708	1.00	16.25
ATOM	1390	CD1	ILE	65	78.087	70.875	59.769	1.00	14.06
ATOM	1391	C	ILE	65	79.729	75.605	59.035	1.00	23.65
ATOM	1392	O	ILE	65	79.123	76.531	58.479	1.00	26.67
ATOM	1393	N	THR	66	80.455	75.899	60.119	1.00	23.04
ATOM	1394	H	THR	66	80.958	75.171	60.524	1.00	0.00
ATOM	1395	CA	THR	66	80.525	77.244	60.665	1.00	20.54
ATOM	1396	CB	THR	66	81.161	77.220	62.037	1.00	25.07
ATOM	1397	OG1	THR	66	82.512	76.718	61.950	1.00	33.54
ATOM	1398	HG1	THR	66	82.484	75.756	62.068	1.00	0.00
ATOM	1399	CG2	THR	66	80.322	76.313	62.956	1.00	26.74
ATOM	1400	C	THR	66	81.288	78.206	59.800	1.00	18.48
ATOM	1401	O	THR	66	80.890	79.364	59.687	1.00	21.50
ATOM	1402	N	GLU	67	82.351	77.809	59.129	1.00	15.71
ATOM	1403	H	GLU	67	82.741	76.945	59.368	1.00	0.00
ATOM	1404	CA	GLU	67	83.030	78.705	58.194	1.00	18.32
ATOM	1405	CB	GLU	67	84.414	78.086	57.866	1.00	22.50
ATOM	1406	CG	GLU	67	85.487	78.159	58.970	1.00	22.14
ATOM	1407	CD	GLU	67	86.936	77.782	58.618	1.00	21.18
ATOM	1408	OE1	GLU	67	87.281	77.495	57.480	1.00	24.37
ATOM	1409	OE2	GLU	67	87.766	77.795	59.514	1.00	18.66
ATOM	1410	C	GLU	67	82.230	79.014	56.887	1.00	19.71
ATOM	1411	O	GLU	67	82.305	80.112	56.304	1.00	18.50
ATOM	1412	N	GLY	68	81.427	78.018	56.425	1.00	19.98
ATOM	1413	H	GLY	68	81.598	77.124	56.785	1.00	0.00
ATOM	1414	CA	GLY	68	80.445	78.167	55.361	1.00	15.48
ATOM	1415	C	GLY	68	79.330	79.110	55.764	1.00	16.79
ATOM	1416	O	GLY	68	79.045	80.122	55.117	1.00	18.82
ATOM	1417	N	ALA	69	78.715	78.849	56.912	1.00	17.97
ATOM	1418	H	ALA	69	78.984	78.035	57.380	1.00	0.00
ATOM	1419	CA	ALA	69	77.677	79.718	57.493	1.00	18.59
ATOM	1420	CB	ALA	69	77.257	79.215	58.860	1.00	14.75
ATOM	1421	C	ALA	69	78.064	81.190	57.669	1.00	21.10
ATOM	1422	O	ALA	69	77.306	82.107	57.321	1.00	24.02
ATOM	1423	N	SER	70	79.275	81.485	58.149	1.00	22.62
ATOM	1424	H	SER	70	79.829	80.759	58.508	1.00	0.00
ATOM	1425	CA	SER	70	79.694	82.886	58.246	1.00	24.11
ATOM	1426	CB	SER	70	81.028	83.020	58.932	1.00	24.37
ATOM	1427	OG	SER	70	81.017	82.382	60.209	1.00	31.83
ATOM	1428	HG	SER	70	81.056	81.422	60.109	1.00	0.00
ATOM	1429	C	SER	70	79.823	83.643	56.929	1.00	25.90
ATOM	1430	O	SER	70	79.634	84.861	56.923	1.00	28.63
ATOM	1431	N	ILE	71	80.142	82.978	55.795	1.00	24.97

33/145

FIGURE 1 (CONT.)

ATOM	1432	H	ILE	71	80.377	82.030	55.891	1.00	0.00
ATOM	1433	CA	ILE	71	80.226	83.596	54.459	1.00	23.41
ATOM	1434	CB	ILE	71	80.903	82.652	53.398	1.00	23.69
ATOM	1435	CG2	ILE	71	80.890	83.341	52.047	1.00	24.89
ATOM	1436	CG1	ILE	71	82.361	82.400	53.671	1.00	19.79
ATOM	1437	CD1	ILE	71	82.817	81.196	52.878	1.00	19.34
ATOM	1438	C	ILE	71	78.839	83.945	53.950	1.00	22.74
ATOM	1439	O	ILE	71	78.606	85.059	53.484	1.00	24.70
ATOM	1440	N	LEU	72	77.920	82.985	54.077	1.00	21.85
ATOM	1441	H	LEU	72	78.234	82.112	54.400	1.00	0.00
ATOM	1442	CA	LEU	72	76.496	83.164	53.743	1.00	20.98
ATOM	1443	CB	LEU	72	75.709	81.895	54.068	1.00	19.13
ATOM	1444	CG	LEU	72	76.266	80.636	53.324	1.00	24.67
ATOM	1445	CD1	LEU	72	75.839	79.326	53.985	1.00	22.09
ATOM	1446	CD2	LEU	72	75.844	80.751	51.863	1.00	21.08
ATOM	1447	C	LEU	72	75.915	84.326	54.524	1.00	21.39
ATOM	1448	O	LEU	72	75.463	85.283	53.923	1.00	20.39
ATOM	1449	N	ARG	73	76.044	84.374	55.851	1.00	22.29
ATOM	1450	H	ARG	73	76.484	83.618	56.297	1.00	0.00
ATOM	1451	CA	ARG	73	75.549	85.486	56.674	1.00	22.78
ATOM	1452	CB	ARG	73	76.063	85.251	58.083	1.00	25.17
ATOM	1453	CG	ARG	73	75.622	86.337	59.052	1.00	24.03
ATOM	1454	CD	ARG	73	76.254	86.153	60.368	1.00	22.43
ATOM	1455	NE	ARG	73	75.660	85.003	61.003	1.00	28.78
ATOM	1456	HE	ARG	73	74.695	84.984	61.166	1.00	0.00
ATOM	1457	CZ	ARG	73	76.403	83.954	61.376	1.00	35.32
ATOM	1458	NH1	ARG	73	75.743	82.933	61.937	1.00	40.90
ATOM	1459	HH11	ARG	73	74.751	82.976	62.052	1.00	0.00
ATOM	1460	HH12	ARG	73	76.247	82.118	62.226	1.00	0.00
ATOM	1461	NH2	ARG	73	77.758	83.888	61.232	1.00	36.08
ATOM	1462	HH21	ARG	73	78.266	84.646	60.824	1.00	0.00
ATOM	1463	HH22	ARG	73	78.246	83.066	61.527	1.00	0.00
ATOM	1464	C	ARG	73	75.880	86.922	56.232	1.00	23.51
ATOM	1465	O	ARG	73	75.124	87.892	56.400	1.00	22.79
ATOM	1466	N	GLN	74	77.068	87.086	55.649	1.00	24.86
ATOM	1467	H	GLN	74	77.650	86.308	55.520	1.00	0.00
ATOM	1468	CA	GLN	74	77.419	88.407	55.160	1.00	26.55
ATOM	1469	CB	GLN	74	78.940	88.474	55.031	1.00	29.60
ATOM	1470	CG	GLN	74	79.810	88.001	56.223	1.00	34.91
ATOM	1471	CD	GLN	74	79.318	88.110	57.691	1.00	38.93
ATOM	1472	OE1	GLN	74	79.577	87.200	58.501	1.00	39.29
ATOM	1473	NE2	GLN	74	78.616	89.147	58.175	1.00	36.05
ATOM	1474	HE21	GLN	74	78.369	89.884	57.589	1.00	0.00
ATOM	1475	HE22	GLN	74	78.390	89.058	59.122	1.00	0.00
ATOM	1476	C	GLN	74	76.719	88.742	53.830	1.00	25.84

FIGURE 1 (CONT.)

ATOM	1477	O	GLN	74	76.447	89.904	53.504	1.00	27.25
ATOM	1478	N	GLU	75	76.368	87.719	53.048	1.00	25.82
ATOM	1479	H	GLU	75	76.539	86.819	53.390	1.00	0.00
ATOM	1480	CA	GLU	75	75.639	87.854	51.783	1.00	24.99
ATOM	1481	CB	GLU	75	75.566	86.508	51.116	1.00	24.81
ATOM	1482	CG	GLU	75	76.953	85.955	50.811	1.00	21.07
ATOM	1483	CD	GLU	75	76.949	84.863	49.767	1.00	17.68
ATOM	1484	OE1	GLU	75	77.514	85.124	48.722	1.00	23.33
ATOM	1485	OE2	GLU	75	76.388	83.788	49.959	1.00	19.85
ATOM	1486	C	GLU	75	74.216	88.435	51.823	1.00	26.11
ATOM	1487	O	GLU	75	73.497	88.298	52.813	1.00	25.53
ATOM	1488	N	LYS	76	73.782	89.120	50.756	1.00	25.59
ATOM	1489	H	LYS	76	74.333	89.103	49.952	1.00	0.00
ATOM	1490	CA	LYS	76	72.494	89.794	50.752	1.00	25.39
ATOM	1491	CB	LYS	76	72.507	90.856	49.672	1.00	29.35
ATOM	1492	CG	LYS	76	73.557	91.959	49.783	1.00	33.02
ATOM	1493	CD	LYS	76	73.713	92.844	48.515	1.00	38.84
ATOM	1494	CE	LYS	76	75.209	93.284	48.340	1.00	42.73
ATOM	1495	NZ	LYS	76	75.481	94.280	47.304	1.00	42.85
ATOM	1496	HZ1	LYS	76	76.496	94.503	47.300	1.00	0.00
ATOM	1497	HZ2	LYS	76	74.950	95.146	47.530	1.00	0.00
ATOM	1498	HZ3	LYS	76	75.199	93.929	46.369	1.00	0.00
ATOM	1499	C	LYS	76	71.308	88.871	50.529	1.00	25.78
ATOM	1500	O	LYS	76	71.465	87.877	49.816	1.00	27.09
ATOM	1501	N	ASN	77	70.103	89.150	51.085	1.00	25.34
ATOM	1502	H	ASN	77	70.083	89.881	51.733	1.00	0.00
ATOM	1503	CA	ASN	77	68.868	88.324	50.899	1.00	23.86
ATOM	1504	CB	ASN	77	67.539	89.041	51.317	1.00	22.89
ATOM	1505	CG	ASN	77	67.204	89.284	52.794	1.00	21.18
ATOM	1506	OD1	ASN	77	67.796	88.765	53.733	1.00	25.75
ATOM	1507	ND2	ASN	77	66.222	90.083	53.123	1.00	16.83
ATOM	1508	HD21	ASN	77	65.671	90.493	52.436	1.00	0.00
ATOM	1509	HD22	ASN	77	66.142	90.275	54.081	1.00	0.00
ATOM	1510	C	ASN	77	68.634	87.908	49.450	1.00	22.54
ATOM	1511	O	ASN	77	68.309	86.774	49.109	1.00	23.17
ATOM	1512	N	LEU	78	68.819	88.919	48.623	1.00	21.52
ATOM	1513	H	LEU	78	69.059	89.780	49.014	1.00	0.00
ATOM	1514	CA	LEU	78	68.790	88.816	47.187	1.00	21.81
ATOM	1515	CB	LEU	78	67.827	89.900	46.711	1.00	22.02
ATOM	1516	CG	LEU	78	67.507	90.136	45.229	1.00	21.03
ATOM	1517	CD1	LEU	78	66.754	88.973	44.588	1.00	13.83
ATOM	1518	CD2	LEU	78	66.662	91.388	45.166	1.00	18.04
ATOM	1519	C	LEU	78	70.224	88.999	46.641	1.00	23.26
ATOM	1520	O	LEU	78	70.851	90.050	46.803	1.00	24.56
ATOM	1521	N	LEU	79	70.849	88.000	46.024	1.00	23.75

35/145

FIGURE 1 (CONT.)

ATOM	1522	H	LEU	79	70.406	87.135	45.993	1.00	0.00
ATOM	1523	CA	LEU	79	72.204	88.139	45.495	1.00	20.55
ATOM	1524	CB	LEU	79	72.832	86.778	45.349	1.00	17.37
ATOM	1525	CG	LEU	79	72.925	85.918	46.576	1.00	17.55
ATOM	1526	CD1	LEU	79	73.075	84.441	46.162	1.00	15.36
ATOM	1527	CD2	LEU	79	74.032	86.484	47.462	1.00	14.33
ATOM	1528	C	LEU	79	72.199	88.815	44.141	1.00	22.27
ATOM	1529	O	LEU	79	71.171	88.812	43.472	1.00	19.98
ATOM	1530	N	ASP	80	73.287	89.431	43.694	1.00	24.45
ATOM	1531	H	ASP	80	74.051	89.517	44.303	1.00	0.00
ATOM	1532	CA	ASP	80	73.296	89.969	42.335	1.00	27.61
ATOM	1533	CB	ASP	80	73.812	91.361	42.182	1.00	30.56
ATOM	1534	CG	ASP	80	73.122	92.378	43.031	1.00	33.32
ATOM	1535	OD1	ASP	80	72.137	92.957	42.548	1.00	37.74
ATOM	1536	OD2	ASP	80	73.601	92.574	44.154	1.00	36.22
ATOM	1537	C	ASP	80	74.307	89.147	41.602	1.00	28.65
ATOM	1538	O	ASP	80	75.508	89.284	41.829	1.00	30.65
ATOM	1539	N	ILE	81	73.860	88.247	40.752	1.00	28.18
ATOM	1540	H	ILE	81	72.901	88.209	40.578	1.00	0.00
ATOM	1541	CA	ILE	81	74.782	87.359	40.081	1.00	26.19
ATOM	1542	CB	ILE	81	74.229	85.929	40.296	1.00	23.56
ATOM	1543	CG2	ILE	81	75.053	84.895	39.544	1.00	23.16
ATOM	1544	CG1	ILE	81	74.273	85.621	41.796	1.00	21.34
ATOM	1545	CD1	ILE	81	73.918	84.178	42.198	1.00	19.01
ATOM	1546	C	ILE	81	75.040	87.673	38.613	1.00	27.80
ATOM	1547	O	ILE	81	74.062	87.788	37.873	1.00	26.93
ATOM	1548	N	ASP	82	76.286	87.859	38.137	1.00	28.35
ATOM	1549	H	ASP	82	77.040	87.865	38.759	1.00	0.00
ATOM	1550	CA	ASP	82	76.494	87.963	36.685	1.00	29.41
ATOM	1551	CB	ASP	82	77.749	88.658	36.277	1.00	33.58
ATOM	1552	CG	ASP	82	77.942	90.007	36.909	1.00	39.71
ATOM	1553	OD1	ASP	82	78.930	90.142	37.642	1.00	41.85
ATOM	1554	OD2	ASP	82	77.117	90.892	36.661	1.00	43.17
ATOM	1555	C	ASP	82	76.603	86.657	35.909	1.00	26.50
ATOM	1556	O	ASP	82	77.108	85.669	36.428	1.00	25.07
ATOM	1557	N	ALA	83	76.116	86.636	34.671	1.00	24.98
ATOM	1558	H	ALA	83	75.691	87.443	34.321	1.00	0.00
ATOM	1559	CA	ALA	83	76.409	85.509	33.782	1.00	25.44
ATOM	1560	CB	ALA	83	75.552	85.497	32.544	1.00	24.97
ATOM	1561	C	ALA	83	77.854	85.618	33.272	1.00	24.70
ATOM	1562	O	ALA	83	78.350	86.751	33.257	1.00	27.83
ATOM	1563	N	PRO	84	78.614	84.591	32.857	1.00	21.31
ATOM	1564	CD	PRO	84	80.056	84.659	32.642	1.00	16.02
ATOM	1565	CA	PRO	84	78.186	83.225	32.760	1.00	19.46
ATOM	1566	CB	PRO	84	79.350	82.557	32.067	1.00	17.97

36/145

FIGURE 1 (CONT.)

ATOM	1567	CG	PRO	84	80.203	83.661	31.539	1.00	14.28
ATOM	1568	C	PRO	84	77.826	82.611	34.112	1.00	21.27
ATOM	1569	O	PRO	84	78.535	82.784	35.097	1.00	20.14
ATOM	1570	N	VAL	85	76.651	81.998	34.206	1.00	21.17
ATOM	1571	H	VAL	85	76.043	82.034	33.438	1.00	0.00
ATOM	1572	CA	VAL	85	76.314	81.221	35.387	1.00	22.34
ATOM	1573	CB	VAL	85	75.217	81.749	36.340	1.00	22.68
ATOM	1574	CG1	VAL	85	75.684	81.438	37.756	1.00	17.16
ATOM	1575	CG2	VAL	85	74.898	83.195	36.092	1.00	26.12
ATOM	1576	C	VAL	85	75.718	79.893	34.952	1.00	23.60
ATOM	1577	O	VAL	85	75.008	79.811	33.942	1.00	24.19
ATOM	1578	N	THR	86	76.070	78.815	35.644	1.00	21.64
ATOM	1579	H	THR	86	76.768	78.890	36.330	1.00	0.00
ATOM	1580	CA	THR	86	75.309	77.614	35.426	1.00	22.02
ATOM	1581	CB	THR	86	76.275	76.374	35.188	1.00	24.41
ATOM	1582	OG1	THR	86	75.561	75.143	35.421	1.00	25.18
ATOM	1583	HG1	THR	86	76.189	74.445	35.636	1.00	0.00
ATOM	1584	CG2	THR	86	77.472	76.498	35.984	1.00	25.54
ATOM	1585	C	THR	86	74.437	77.531	36.678	1.00	19.18
ATOM	1586	O	THR	86	74.858	77.803	37.803	1.00	19.84
ATOM	1587	N	VAL	87	73.136	77.465	36.426	1.00	15.26
ATOM	1588	H	VAL	87	72.868	77.494	35.491	1.00	0.00
ATOM	1589	CA	VAL	87	72.128	77.365	37.469	1.00	14.68
ATOM	1590	CB	VAL	87	70.931	78.225	37.064	1.00	13.83
ATOM	1591	CG1	VAL	87	69.913	78.280	38.179	1.00	7.16
ATOM	1592	CG2	VAL	87	71.449	79.597	36.662	1.00	8.43
ATOM	1593	C	VAL	87	71.688	75.916	37.758	1.00	16.39
ATOM	1594	O	VAL	87	71.408	75.110	36.864	1.00	18.18
ATOM	1595	N	CYS	88	71.694	75.525	39.025	1.00	16.75
ATOM	1596	H	CYS	88	71.965	76.173	39.707	1.00	0.00
ATOM	1597	CA	CYS	88	71.396	74.163	39.404	1.00	14.45
ATOM	1598	CB	CYS	88	72.513	73.600	40.152	1.00	12.05
ATOM	1599	SG	CYS	88	73.849	73.692	38.981	1.00	12.68
ATOM	1600	C	CYS	88	70.173	74.029	40.252	1.00	17.38
ATOM	1601	O	CYS	88	69.947	74.877	41.117	1.00	23.03
ATOM	1602	N	GLY	89	69.359	73.008	40.017	1.00	15.87
ATOM	1603	H	GLY	89	69.631	72.353	39.347	1.00	0.00
ATOM	1604	CA	GLY	89	68.149	72.819	40.771	1.00	12.25
ATOM	1605	C	GLY	89	68.367	71.846	41.899	1.00	13.66
ATOM	1606	O	GLY	89	69.491	71.552	42.273	1.00	17.05
ATOM	1607	N	ASP	90	67.293	71.289	42.422	1.00	13.25
ATOM	1608	H	ASP	90	66.460	71.482	41.955	1.00	0.00
ATOM	1609	CA	ASP	90	67.282	70.439	43.627	1.00	14.52
ATOM	1610	CB	ASP	90	65.905	69.777	43.814	1.00	17.28
ATOM	1611	CG	ASP	90	64.717	70.748	43.977	1.00	23.77

37/145

FIGURE 1 (CONT.)

ATOM	1612	OD1	ASP	90	63.699	70.300	44.481	1.00	23.87
ATOM	1613	OD2	ASP	90	64.786	71.939	43.625	1.00	24.07
ATOM	1614	C	ASP	90	68.295	69.332	43.670	1.00	13.73
ATOM	1615	O	ASP	90	68.330	68.597	42.702	1.00	17.62
ATOM	1616	N	ILE	91	69.067	69.157	44.731	1.00	12.91
ATOM	1617	H	ILE	91	69.034	69.865	45.407	1.00	0.00
ATOM	1618	CA	ILE	91	70.079	68.099	44.814	1.00	13.40
ATOM	1619	CB	ILE	91	71.428	68.756	45.405	1.00	11.92
ATOM	1620	CG2	ILE	91	72.500	67.746	45.849	1.00	8.36
ATOM	1621	CG1	ILE	91	72.027	69.633	44.297	1.00	12.03
ATOM	1622	CD1	ILE	91	72.515	68.888	43.007	1.00	4.73
ATOM	1623	C	ILE	91	69.584	66.916	45.652	1.00	16.29
ATOM	1624	O	ILE	91	69.777	65.741	45.353	1.00	18.91
ATOM	1625	N	HIS	92	68.913	67.220	46.762	1.00	15.90
ATOM	1626	H	HIS	92	68.792	68.172	46.911	1.00	0.00
ATOM	1627	CA	HIS	92	68.393	66.250	47.715	1.00	13.28
ATOM	1628	CB	HIS	92	67.110	65.676	47.195	1.00	11.50
ATOM	1629	CG	HIS	92	65.998	66.657	47.467	1.00	12.28
ATOM	1630	CD2	HIS	92	65.183	67.171	46.511	1.00	13.22
ATOM	1631	ND1	HIS	92	65.643	67.188	48.616	1.00	13.26
ATOM	1632	HD1	HIS	92	66.060	67.003	49.493	1.00	0.00
ATOM	1633	CE1	HIS	92	64.656	67.998	48.392	1.00	12.51
ATOM	1634	NE2	HIS	92	64.388	67.982	47.125	1.00	13.73
ATOM	1635	HE2	HIS	92	63.547	68.250	46.715	1.00	0.00
ATOM	1636	C	HIS	92	69.266	65.093	48.170	1.00	15.16
ATOM	1637	O	HIS	92	68.983	63.924	47.918	1.00	17.65
ATOM	1638	N	GLY	93	70.383	65.310	48.837	1.00	12.61
ATOM	1639	H	GLY	93	70.746	66.205	48.938	1.00	0.00
ATOM	1640	CA	GLY	93	71.102	64.180	49.364	1.00	11.45
ATOM	1641	C	GLY	93	71.723	63.240	48.359	1.00	9.28
ATOM	1642	O	GLY	93	72.405	62.292	48.738	1.00	10.05
ATOM	1643	N	GLN	94	71.547	63.448	47.075	1.00	11.96
ATOM	1644	H	GLN	94	70.956	64.171	46.784	1.00	0.00
ATOM	1645	CA	GLN	94	72.143	62.570	46.073	1.00	14.58
ATOM	1646	CB	GLN	94	71.283	62.515	44.830	1.00	15.52
ATOM	1647	CG	GLN	94	69.825	62.227	45.107	1.00	18.07
ATOM	1648	CD	GLN	94	68.921	62.134	43.892	1.00	17.85
ATOM	1649	OE1	GLN	94	67.731	62.345	44.020	1.00	20.75
ATOM	1650	NE2	GLN	94	69.290	61.786	42.677	1.00	17.16
ATOM	1651	HE21	GLN	94	70.227	61.615	42.498	1.00	0.00
ATOM	1652	HE22	GLN	94	68.560	61.705	42.026	1.00	0.00
ATOM	1653	C	GLN	94	73.533	63.036	45.682	1.00	15.97
ATOM	1654	O	GLN	94	73.841	63.394	44.542	1.00	16.30
ATOM	1655	N	PHE	95	74.422	62.944	46.667	1.00	18.16
ATOM	1656	H	PHE	95	74.079	62.633	47.535	1.00	0.00

FIGURE 1 (CONT.)

ATOM	1657	CA	PHE	95	75.823	63.340	46.556	1.00	18.64
ATOM	1658	CB	PHE	95	76.586	62.899	47.792	1.00	18.42
ATOM	1659	CG	PHE	95	78.090	63.135	47.750	1.00	16.62
ATOM	1660	CD1	PHE	95	78.954	62.043	47.620	1.00	17.26
ATOM	1661	CD2	PHE	95	78.585	64.430	47.866	1.00	15.80
ATOM	1662	CE1	PHE	95	80.317	62.259	47.606	1.00	16.94
ATOM	1663	CE2	PHE	95	79.951	64.633	47.854	1.00	14.48
ATOM	1664	CZ	PHE	95	80.813	63.556	47.724	1.00	14.67
ATOM	1665	C	PHE	95	76.520	62.771	45.349	1.00	19.39
ATOM	1666	O	PHE	95	77.258	63.472	44.658	1.00	20.09
ATOM	1667	N	PHE	96	76.255	61.498	45.028	1.00	19.87
ATOM	1668	H	PHE	96	75.670	60.957	45.597	1.00	0.00
ATOM	1669	CA	PHE	96	76.970	60.938	43.884	1.00	18.26
ATOM	1670	CB	PHE	96	76.895	59.466	43.968	1.00	17.59
ATOM	1671	CG	PHE	96	77.701	58.971	45.176	1.00	22.20
ATOM	1672	CD1	PHE	96	77.076	58.838	46.442	1.00	21.86
ATOM	1673	CD2	PHE	96	79.040	58.590	45.010	1.00	18.55
ATOM	1674	CE1	PHE	96	77.783	58.317	47.530	1.00	21.32
ATOM	1675	CE2	PHE	96	79.721	58.070	46.110	1.00	20.98
ATOM	1676	CZ	PHE	96	79.108	57.931	47.359	1.00	19.11
ATOM	1677	C	PHE	96	76.502	61.422	42.534	1.00	18.25
ATOM	1678	O	PHE	96	77.204	61.284	41.537	1.00	21.63
ATOM	1679	N	ASP	97	75.339	62.082	42.545	1.00	15.89
ATOM	1680	H	ASP	97	74.828	62.091	43.378	1.00	0.00
ATOM	1681	CA	ASP	97	74.792	62.741	41.390	1.00	13.39
ATOM	1682	CB	ASP	97	73.286	62.676	41.455	1.00	14.76
ATOM	1683	CG	ASP	97	72.744	61.319	41.043	1.00	14.79
ATOM	1684	OD1	ASP	97	73.032	60.917	39.924	1.00	19.87
ATOM	1685	OD2	ASP	97	72.046	60.655	41.808	1.00	16.12
ATOM	1686	C	ASP	97	75.283	64.171	41.385	1.00	13.61
ATOM	1687	O	ASP	97	75.429	64.787	40.341	1.00	15.27
ATOM	1688	N	LEU	98	75.630	64.744	42.534	1.00	14.05
ATOM	1689	H	LEU	98	75.316	64.329	43.365	1.00	0.00
ATOM	1690	CA	LEU	98	76.304	66.052	42.602	1.00	12.58
ATOM	1691	CB	LEU	98	76.565	66.485	44.003	1.00	10.02
ATOM	1692	CG	LEU	98	76.303	67.859	44.588	1.00	12.48
ATOM	1693	CD1	LEU	98	77.375	68.107	45.682	1.00	6.02
ATOM	1694	CD2	LEU	98	76.321	68.923	43.512	1.00	9.01
ATOM	1695	C	LEU	98	77.669	65.954	41.958	1.00	13.11
ATOM	1696	O	LEU	98	78.171	66.880	41.365	1.00	15.78
ATOM	1697	N	MET	99	78.365	64.833	42.069	1.00	16.53
ATOM	1698	H	MET	99	78.009	64.164	42.690	1.00	0.00
ATOM	1699	CA	MET	99	79.672	64.637	41.418	1.00	17.92
ATOM	1700	CB	MET	99	80.226	63.278	41.863	1.00	15.18
ATOM	1701	CG	MET	99	80.244	63.158	43.369	1.00	11.83

FIGURE 1 (CONT.)

ATOM	1702	SD	MET	99	81.362	64.386	44.042	1.00	19.23
ATOM	1703	CE	MET	99	80.423	65.836	44.411	1.00	14.17
ATOM	1704	C	MET	99	79.510	64.720	39.887	1.00	19.73
ATOM	1705	O	MET	99	80.187	65.485	39.183	1.00	20.40
ATOM	1706	N	LYS	100	78.489	64.022	39.377	1.00	19.63
ATOM	1707	H	LYS	100	78.025	63.371	39.939	1.00	0.00
ATOM	1708	CA	LYS	100	78.141	64.164	37.978	1.00	19.81
ATOM	1709	CB	LYS	100	76.978	63.257	37.699	1.00	18.14
ATOM	1710	CG	LYS	100	76.737	63.170	36.221	1.00	20.40
ATOM	1711	CD	LYS	100	77.992	62.690	35.520	1.00	24.15
ATOM	1712	CE	LYS	100	77.647	62.595	34.053	1.00	29.22
ATOM	1713	NZ	LYS	100	78.812	62.204	33.278	1.00	33.01
ATOM	1714	HZ1	LYS	100	79.559	62.910	33.419	1.00	0.00
ATOM	1715	HZ2	LYS	100	78.557	62.171	32.269	1.00	0.00
ATOM	1716	HZ3	LYS	100	79.146	61.267	33.583	1.00	0.00
ATOM	1717	C	LYS	100	77.819	65.614	37.569	1.00	19.62
ATOM	1718	O	LYS	100	78.354	66.153	36.606	1.00	20.04
ATOM	1719	N	LEU	101	77.007	66.317	38.323	1.00	18.30
ATOM	1720	H	LEU	101	76.591	65.855	39.083	1.00	0.00
ATOM	1721	CA	LEU	101	76.644	67.687	38.044	1.00	18.00
ATOM	1722	CB	LEU	101	75.813	68.193	39.235	1.00	14.61
ATOM	1723	CG	LEU	101	75.272	69.575	39.169	1.00	13.38
ATOM	1724	CD1	LEU	101	73.977	69.493	39.892	1.00	12.35
ATOM	1725	CD2	LEU	101	76.209	70.632	39.714	1.00	8.60
ATOM	1726	C	LEU	101	77.868	68.575	37.805	1.00	20.00
ATOM	1727	O	LEU	101	77.894	69.293	36.803	1.00	21.46
ATOM	1728	N	PHE	102	78.894	68.563	38.678	1.00	18.83
ATOM	1729	H	PHE	102	78.817	68.004	39.482	1.00	0.00
ATOM	1730	CA	PHE	102	80.060	69.396	38.449	1.00	16.56
ATOM	1731	CB	PHE	102	80.866	69.367	39.696	1.00	16.41
ATOM	1732	CG	PHE	102	80.301	70.135	40.878	1.00	16.22
ATOM	1733	CD1	PHE	102	80.085	71.511	40.803	1.00	17.75
ATOM	1734	CD2	PHE	102	80.031	69.471	42.067	1.00	18.34
ATOM	1735	CE1	PHE	102	79.604	72.218	41.905	1.00	14.49
ATOM	1736	CE2	PHE	102	79.547	70.195	43.178	1.00	22.31
ATOM	1737	CZ	PHE	102	79.333	71.568	43.096	1.00	18.01
ATOM	1738	C	PHE	102	80.848	68.883	37.223	1.00	19.71
ATOM	1739	O	PHE	102	81.497	69.681	36.536	1.00	21.54
ATOM	1740	N	GLU	103	80.843	67.572	36.869	1.00	19.67
ATOM	1741	H	GLU	103	80.484	66.921	37.510	1.00	0.00
ATOM	1742	CA	GLU	103	81.338	67.124	35.553	1.00	20.12
ATOM	1743	CB	GLU	103	81.128	65.659	35.285	1.00	22.22
ATOM	1744	CG	GLU	103	81.921	64.503	35.857	1.00	29.90
ATOM	1745	CD	GLU	103	81.688	63.175	35.084	1.00	33.72
ATOM	1746	OE1	GLU	103	81.737	62.114	35.702	1.00	35.67

FIGURE 1 (CONT.)

ATOM	1747	OE2	GLU	103	81.459	63.165	33.865	1.00	34.36
ATOM	1748	C	GLU	103	80.537	67.822	34.423	1.00	19.59
ATOM	1749	O	GLU	103	81.074	68.522	33.594	1.00	21.84
ATOM	1750	N	VAL	104	79.214	67.758	34.336	1.00	20.28
ATOM	1751	H	VAL	104	78.769	67.278	35.065	1.00	0.00
ATOM	1752	CA	VAL	104	78.395	68.376	33.281	1.00	19.91
ATOM	1753	CB	VAL	104	76.940	67.814	33.542	1.00	18.88
ATOM	1754	CG1	VAL	104	75.877	68.524	32.752	1.00	17.73
ATOM	1755	CG2	VAL	104	76.911	66.346	33.129	1.00	13.28
ATOM	1756	C	VAL	104	78.470	69.925	33.222	1.00	22.25
ATOM	1757	O	VAL	104	78.621	70.536	32.152	1.00	25.12
ATOM	1758	N	GLY	105	78.342	70.595	34.375	1.00	21.92
ATOM	1759	H	GLY	105	78.239	70.055	35.175	1.00	0.00
ATOM	1760	CA	GLY	105	78.349	72.055	34.493	1.00	20.15
ATOM	1761	C	GLY	105	79.721	72.695	34.376	1.00	21.14
ATOM	1762	O	GLY	105	79.909	73.793	33.843	1.00	24.50
ATOM	1763	N	GLY	106	80.722	71.992	34.855	1.00	19.70
ATOM	1764	H	GLY	106	80.541	71.105	35.223	1.00	0.00
ATOM	1765	CA	GLY	106	82.070	72.477	34.805	1.00	20.01
ATOM	1766	C	GLY	106	82.725	72.532	36.183	1.00	23.34
ATOM	1767	O	GLY	106	82.087	72.343	37.210	1.00	25.07
ATOM	1768	N	SER	107	84.024	72.810	36.278	1.00	24.17
ATOM	1769	H	SER	107	84.500	72.996	35.447	1.00	0.00
ATOM	1770	CA	SER	107	84.702	72.927	37.569	1.00	20.74
ATOM	1771	CB	SER	107	86.199	73.032	37.430	1.00	19.20
ATOM	1772	OG	SER	107	86.814	72.822	38.691	1.00	20.71
ATOM	1773	HG	SER	107	87.753	72.653	38.534	1.00	0.00
ATOM	1774	C	SER	107	84.296	74.164	38.327	1.00	18.27
ATOM	1775	O	SER	107	84.271	75.218	37.701	1.00	18.11
ATOM	1776	N	PRO	108	84.061	74.158	39.647	1.00	17.40
ATOM	1777	CD	PRO	108	83.900	72.972	40.483	1.00	15.32
ATOM	1778	CA	PRO	108	83.954	75.374	40.440	1.00	16.47
ATOM	1779	CB	PRO	108	83.676	74.853	41.811	1.00	11.22
ATOM	1780	CG	PRO	108	83.010	73.558	41.531	1.00	11.77
ATOM	1781	C	PRO	108	85.245	76.206	40.326	1.00	20.15
ATOM	1782	O	PRO	108	85.260	77.421	40.520	1.00	24.43
ATOM	1783	N	ALA	109	86.375	75.558	39.997	1.00	20.60
ATOM	1784	H	ALA	109	86.321	74.582	39.932	1.00	0.00
ATOM	1785	CA	ALA	109	87.672	76.180	39.790	1.00	18.81
ATOM	1786	CB	ALA	109	88.676	75.214	39.285	1.00	17.25
ATOM	1787	C	ALA	109	87.642	77.268	38.759	1.00	21.06
ATOM	1788	O	ALA	109	88.407	78.227	38.825	1.00	24.57
ATOM	1789	N	ASN	110	86.749	77.090	37.796	1.00	23.02
ATOM	1790	H	ASN	110	86.217	76.271	37.802	1.00	0.00
ATOM	1791	CA	ASN	110	86.567	78.077	36.743	1.00	24.98

41/145

FIGURE 1 (CONT.)

ATOM	1792	CB	ASN	110	87.469	77.717	35.549	1.00	28.49
ATOM	1793	CG	ASN	110	87.074	76.397	34.963	1.00	29.08
ATOM	1794	OD1	ASN	110	87.585	75.380	35.387	1.00	34.13
ATOM	1795	ND2	ASN	110	86.094	76.283	34.101	1.00	29.72
ATOM	1796	HD21	ASN	110	85.583	77.083	33.870	1.00	0.00
ATOM	1797	HD22	ASN	110	85.952	75.387	33.757	1.00	0.00
ATOM	1798	C	ASN	110	85.154	78.303	36.217	1.00	23.35
ATOM	1799	O	ASN	110	84.974	78.860	35.138	1.00	23.53
ATOM	1800	N	THR	111	84.124	77.815	36.880	1.00	23.28
ATOM	1801	H	THR	111	84.277	77.273	37.680	1.00	0.00
ATOM	1802	CA	THR	111	82.755	78.005	36.402	1.00	20.55
ATOM	1803	CB	THR	111	82.011	76.687	36.078	1.00	17.61
ATOM	1804	OG1	THR	111	82.877	75.842	35.325	1.00	16.07
ATOM	1805	HG1	THR	111	82.307	75.264	34.803	1.00	0.00
ATOM	1806	CG2	THR	111	80.752	76.950	35.283	1.00	11.55
ATOM	1807	C	THR	111	81.937	78.687	37.471	1.00	22.32
ATOM	1808	O	THR	111	81.986	78.286	38.637	1.00	25.14
ATOM	1809	N	ARG	112	81.195	79.737	37.145	1.00	23.02
ATOM	1810	H	ARG	112	81.286	80.143	36.261	1.00	0.00
ATOM	1811	CA	ARG	112	80.306	80.324	38.136	1.00	22.16
ATOM	1812	CB	ARG	112	79.817	81.625	37.622	1.00	25.25
ATOM	1813	CG	ARG	112	80.225	82.882	38.331	1.00	31.08
ATOM	1814	CD	ARG	112	80.239	84.030	37.276	1.00	33.63
ATOM	1815	NE	ARG	112	80.445	85.274	37.972	1.00	38.57
ATOM	1816	HE	ARG	112	81.298	85.749	37.885	1.00	0.00
ATOM	1817	CZ	ARG	112	79.479	85.769	38.771	1.00	43.88
ATOM	1818	NH1	ARG	112	79.721	86.878	39.521	1.00	45.08
ATOM	1819	HH11	ARG	112	80.632	87.290	39.514	1.00	0.00
ATOM	1820	HH12	ARG	112	79.032	87.204	40.168	1.00	0.00
ATOM	1821	NH2	ARG	112	78.261	85.187	38.818	1.00	40.87
ATOM	1822	HH21	ARG	112	78.059	84.369	38.281	1.00	0.00
ATOM	1823	HH22	ARG	112	77.583	85.541	39.462	1.00	0.00
ATOM	1824	C	ARG	112	79.108	79.397	38.378	1.00	22.37
ATOM	1825	O	ARG	112	78.500	78.882	37.426	1.00	19.09
ATOM	1826	N	TYR	113	78.756	79.162	39.645	1.00	20.28
ATOM	1827	H	TYR	113	79.331	79.554	40.332	1.00	0.00
ATOM	1828	CA	TYR	113	77.600	78.369	40.047	1.00	16.36
ATOM	1829	CB	TYR	113	78.073	77.219	40.859	1.00	15.16
ATOM	1830	CG	TYR	113	78.478	76.079	39.948	1.00	19.88
ATOM	1831	CD1	TYR	113	77.446	75.310	39.387	1.00	17.88
ATOM	1832	CE1	TYR	113	77.767	74.240	38.558	1.00	17.80
ATOM	1833	CD2	TYR	113	79.830	75.783	39.679	1.00	15.86
ATOM	1834	CE2	TYR	113	80.131	74.702	38.848	1.00	14.15
ATOM	1835	CZ	TYR	113	79.101	73.947	38.299	1.00	13.05
ATOM	1836	OH	TYR	113	79.351	72.878	37.472	1.00	16.26

42/145

FIGURE 1 (CONT.)

ATOM	1837	HH	TYR	113	80.296	72.683	37.479	1.00	0.00
ATOM	1838	C	TYR	113	76.471	79.016	40.810	1.00	14.43
ATOM	1839	O	TYR	113	76.731	79.848	41.645	1.00	18.02
ATOM	1840	N	LEU	114	75.196	78.751	40.587	1.00	16.97
ATOM	1841	H	LEU	114	74.982	78.229	39.780	1.00	0.00
ATOM	1842	CA	LEU	114	74.086	79.231	41.427	1.00	14.11
ATOM	1843	CB	LEU	114	73.108	80.049	40.684	1.00	13.97
ATOM	1844	CG	LEU	114	72.360	81.262	41.192	1.00	16.23
ATOM	1845	CD1	LEU	114	71.386	81.615	40.082	1.00	18.72
ATOM	1846	CD2	LEU	114	71.585	81.043	42.451	1.00	14.39
ATOM	1847	C	LEU	114	73.349	77.984	41.810	1.00	15.05
ATOM	1848	O	LEU	114	72.980	77.186	40.945	1.00	18.40
ATOM	1849	N	PHE	115	73.120	77.708	43.071	1.00	15.74
ATOM	1850	H	PHE	115	73.433	78.345	43.737	1.00	0.00
ATOM	1851	CA	PHE	115	72.364	76.520	43.495	1.00	12.20
ATOM	1852	CB	PHE	115	73.139	75.702	44.505	1.00	9.15
ATOM	1853	CG	PHE	115	74.183	74.751	43.931	1.00	4.55
ATOM	1854	CD1	PHE	115	75.449	75.207	43.588	1.00	6.18
ATOM	1855	CD2	PHE	115	73.838	73.419	43.715	1.00	2.77
ATOM	1856	CE1	PHE	115	76.369	74.322	43.011	1.00	5.39
ATOM	1857	CE2	PHE	115	74.753	72.546	43.142	1.00	2.48
ATOM	1858	CZ	PHE	115	76.021	72.997	42.786	1.00	2.34
ATOM	1859	C	PHE	115	71.060	76.960	44.139	1.00	13.75
ATOM	1860	O	PHE	115	71.010	77.730	45.101	1.00	16.34
ATOM	1861	N	LEU	116	69.957	76.534	43.580	1.00	13.45
ATOM	1862	H	LEU	116	70.039	75.951	42.791	1.00	0.00
ATOM	1863	CA	LEU	116	68.635	76.929	44.041	1.00	15.21
ATOM	1864	CB	LEU	116	67.786	76.842	42.757	1.00	13.18
ATOM	1865	CG	LEU	116	67.560	78.096	41.935	1.00	11.70
ATOM	1866	CD1	LEU	116	68.781	78.875	41.691	1.00	7.70
ATOM	1867	CD2	LEU	116	67.062	77.656	40.587	1.00	14.61
ATOM	1868	C	LEU	116	67.983	76.218	45.262	1.00	17.06
ATOM	1869	O	LEU	116	66.756	76.024	45.399	1.00	19.44
ATOM	1870	N	GLY	117	68.748	75.813	46.260	1.00	17.13
ATOM	1871	H	GLY	117	69.704	76.038	46.230	1.00	0.00
ATOM	1872	CA	GLY	117	68.179	75.124	47.412	1.00	13.85
ATOM	1873	C	GLY	117	67.935	73.624	47.229	1.00	15.63
ATOM	1874	O	GLY	117	68.087	72.979	46.193	1.00	16.84
ATOM	1875	N	ASP	118	67.377	73.091	48.305	1.00	15.22
ATOM	1876	H	ASP	118	67.066	73.755	48.941	1.00	0.00
ATOM	1877	CA	ASP	118	67.129	71.680	48.533	1.00	16.20
ATOM	1878	CB	ASP	118	65.900	71.239	47.743	1.00	15.43
ATOM	1879	CG	ASP	118	64.573	71.648	48.382	1.00	17.15
ATOM	1880	OD1	ASP	118	64.547	72.520	49.249	1.00	15.52
ATOM	1881	OD2	ASP	118	63.546	71.092	47.997	1.00	18.50

43/145

FIGURE 1 (CONT.)

ATOM	1882	C	ASP	118	68.276	70.727	48.276	1.00	16.53
ATOM	1883	O	ASP	118	68.290	69.887	47.380	1.00	20.09
ATOM	1884	N	TYR	119	69.247	70.916	49.161	1.00	14.12
ATOM	1885	H	TYR	119	69.219	71.743	49.671	1.00	0.00
ATOM	1886	CA	TYR	119	70.481	70.126	49.203	1.00	14.00
ATOM	1887	CB	TYR	119	71.592	70.963	49.870	1.00	13.49
ATOM	1888	CG	TYR	119	71.721	72.370	49.313	1.00	12.23
ATOM	1889	CD1	TYR	119	72.067	72.530	47.980	1.00	7.89
ATOM	1890	CE1	TYR	119	72.115	73.800	47.456	1.00	11.16
ATOM	1891	CD2	TYR	119	71.431	73.485	50.132	1.00	13.37
ATOM	1892	CE2	TYR	119	71.472	74.778	49.603	1.00	11.79
ATOM	1893	CZ	TYR	119	71.813	74.912	48.255	1.00	13.58
ATOM	1894	OH	TYR	119	71.802	76.155	47.661	1.00	16.18
ATOM	1895	HH	TYR	119	71.375	76.769	48.279	1.00	0.00
ATOM	1896	C	TYR	119	70.360	68.810	49.963	1.00	13.10
ATOM	1897	O	TYR	119	71.053	67.826	49.772	1.00	10.98
ATOM	1898	N	VAL	120	69.351	68.879	50.816	1.00	14.82
ATOM	1899	H	VAL	120	68.776	69.659	50.765	1.00	0.00
ATOM	1900	CA	VAL	120	69.089	67.943	51.895	1.00	15.66
ATOM	1901	CB	VAL	120	69.367	68.855	53.106	1.00	15.80
ATOM	1902	CG1	VAL	120	68.128	69.002	53.966	1.00	16.16
ATOM	1903	CG2	VAL	120	70.592	68.365	53.791	1.00	11.17
ATOM	1904	C	VAL	120	67.717	67.241	51.868	1.00	18.38
ATOM	1905	O	VAL	120	66.727	67.728	51.273	1.00	18.49
ATOM	1906	N	ASP	121	67.695	66.111	52.586	1.00	17.33
ATOM	1907	H	ASP	121	68.567	65.849	52.959	1.00	0.00
ATOM	1908	CA	ASP	121	66.582	65.180	52.724	1.00	16.76
ATOM	1909	CB	ASP	121	65.274	65.871	53.025	1.00	13.45
ATOM	1910	CG	ASP	121	65.214	66.496	54.393	1.00	16.45
ATOM	1911	OD1	ASP	121	64.686	67.603	54.514	1.00	18.01
ATOM	1912	OD2	ASP	121	65.666	65.858	55.339	1.00	14.32
ATOM	1913	C	ASP	121	66.302	64.279	51.539	1.00	18.09
ATOM	1914	O	ASP	121	66.669	64.591	50.412	1.00	22.54
ATOM	1915	N	ARG	122	65.611	63.165	51.734	1.00	18.16
ATOM	1916	H	ARG	122	65.410	62.918	52.664	1.00	0.00
ATOM	1917	CA	ARG	122	65.257	62.206	50.687	1.00	17.31
ATOM	1918	CB	ARG	122	64.570	62.883	49.448	1.00	17.39
ATOM	1919	CG	ARG	122	63.269	63.530	49.941	1.00	20.48
ATOM	1920	CD	ARG	122	61.987	63.209	49.161	1.00	24.78
ATOM	1921	NE	ARG	122	60.822	64.081	49.397	1.00	27.96
ATOM	1922	HE	ARG	122	59.951	63.654	49.526	1.00	0.00
ATOM	1923	CZ	ARG	122	60.888	65.436	49.456	1.00	26.84
ATOM	1924	NH1	ARG	122	59.796	66.186	49.684	1.00	22.77
ATOM	1925	HH11	ARG	122	58.908	65.743	49.816	1.00	0.00
ATOM	1926	HH12	ARG	122	59.873	67.182	49.720	1.00	0.00

FIGURE 1 (CONT.)

ATOM	1927	NH2	ARG	122	62.044	66.089	49.303	1.00	25.45
ATOM	1928	HH21	ARG	122	62.888	65.600	49.095	1.00	0.00
ATOM	1929	HH22	ARG	122	62.060	67.084	49.366	1.00	0.00
ATOM	1930	C	ARG	122	66.459	61.421	50.234	1.00	17.09
ATOM	1931	O	ARG	122	66.411	60.201	50.375	1.00	18.20
ATOM	1932	N	GLY	123	67.560	61.981	49.737	1.00	15.89
ATOM	1933	H	GLY	123	67.578	62.949	49.574	1.00	0.00
ATOM	1934	CA	GLY	123	68.712	61.165	49.384	1.00	12.80
ATOM	1935	C	GLY	123	69.512	60.854	50.626	1.00	13.10
ATOM	1936	O	GLY	123	69.685	61.708	51.483	1.00	15.67
ATOM	1937	N	TYR	124	70.033	59.664	50.845	1.00	14.89
ATOM	1938	H	TYR	124	69.808	58.979	50.196	1.00	0.00
ATOM	1939	CA	TYR	124	70.784	59.334	52.065	1.00	16.07
ATOM	1940	CB	TYR	124	70.618	57.808	52.242	1.00	17.64
ATOM	1941	CG	TYR	124	69.255	57.387	52.810	1.00	16.47
ATOM	1942	CD1	TYR	124	69.095	56.132	53.405	1.00	13.81
ATOM	1943	CE1	TYR	124	67.875	55.763	53.951	1.00	14.96
ATOM	1944	CD2	TYR	124	68.162	58.268	52.767	1.00	17.78
ATOM	1945	CE2	TYR	124	66.931	57.913	53.305	1.00	18.15
ATOM	1946	CZ	TYR	124	66.811	56.665	53.887	1.00	18.05
ATOM	1947	OH	TYR	124	65.587	56.334	54.394	1.00	26.08
ATOM	1948	HH	TYR	124	64.934	56.923	54.001	1.00	0.00
ATOM	1949	C	TYR	124	72.263	59.780	52.199	1.00	15.51
ATOM	1950	O	TYR	124	73.017	59.427	53.095	1.00	15.09
ATOM	1951	N	PHE	125	72.696	60.665	51.320	1.00	15.38
ATOM	1952	H	PHE	125	72.099	60.903	50.581	1.00	0.00
ATOM	1953	CA	PHE	125	74.028	61.230	51.326	1.00	15.32
ATOM	1954	CB	PHE	125	74.742	60.831	50.046	1.00	14.98
ATOM	1955	CG	PHE	125	74.782	59.307	49.878	1.00	15.01
ATOM	1956	CD1	PHE	125	75.624	58.531	50.693	1.00	16.18
ATOM	1957	CD2	PHE	125	73.960	58.687	48.942	1.00	10.27
ATOM	1958	CE1	PHE	125	75.646	57.135	50.573	1.00	14.84
ATOM	1959	CE2	PHE	125	73.994	57.299	48.837	1.00	13.76
ATOM	1960	CZ	PHE	125	74.828	56.518	49.640	1.00	12.07
ATOM	1961	C	PHE	125	73.930	62.743	51.430	1.00	15.30
ATOM	1962	O	PHE	125	74.737	63.480	50.899	1.00	19.01
ATOM	1963	N	SER	126	73.001	63.272	52.222	1.00	16.48
ATOM	1964	H	SER	126	72.400	62.622	52.641	1.00	0.00
ATOM	1965	CA	SER	126	72.759	64.711	52.392	1.00	15.03
ATOM	1966	CB	SER	126	71.399	65.006	53.062	1.00	16.95
ATOM	1967	OG	SER	126	70.201	64.599	52.372	1.00	19.04
ATOM	1968	HG	SER	126	70.186	63.647	52.166	1.00	0.00
ATOM	1969	C	SER	126	73.776	65.476	53.190	1.00	15.27
ATOM	1970	O	SER	126	73.987	66.656	52.925	1.00	14.34
ATOM	1971	N	ILE	127	74.469	64.868	54.175	1.00	17.67

45/145

FIGURE 1 (CONT.)

ATOM	1972	H	ILE	127	74.196	63.981	54.462	1.00	0.00
ATOM	1973	CA	ILE	127	75.538	65.608	54.887	1.00	15.57
ATOM	1974	CB	ILE	127	75.837	64.932	56.314	1.00	13.45
ATOM	1975	CG2	ILE	127	76.546	63.605	56.251	1.00	10.69
ATOM	1976	CG1	ILE	127	76.746	65.842	57.079	1.00	13.34
ATOM	1977	CD1	ILE	127	76.262	67.292	57.232	1.00	13.82
ATOM	1978	C	ILE	127	76.788	65.683	53.996	1.00	17.31
ATOM	1979	O	ILE	127	77.476	66.701	54.067	1.00	18.98
ATOM	1980	N	GLU	128	77.089	64.715	53.084	1.00	14.23
ATOM	1981	H	GLU	128	76.523	63.923	53.046	1.00	0.00
ATOM	1982	CA	GLU	128	78.206	64.856	52.159	1.00	12.73
ATOM	1983	CB	GLU	128	78.430	63.547	51.441	1.00	15.92
ATOM	1984	CG	GLU	128	78.872	62.302	52.254	1.00	14.73
ATOM	1985	CD	GLU	128	77.809	61.328	52.806	1.00	20.61
ATOM	1986	OE1	GLU	128	76.707	61.738	53.207	1.00	20.45
ATOM	1987	OE2	GLU	128	78.105	60.128	52.868	1.00	22.71
ATOM	1988	C	GLU	128	77.942	65.975	51.136	1.00	16.06
ATOM	1989	O	GLU	128	78.840	66.702	50.695	1.00	17.48
ATOM	1990	N	CYS	129	76.683	66.190	50.730	1.00	17.79
ATOM	1991	H	CYS	129	76.024	65.486	50.906	1.00	0.00
ATOM	1992	CA	CYS	129	76.314	67.348	49.893	1.00	17.59
ATOM	1993	CB	CYS	129	74.874	67.344	49.351	1.00	14.57
ATOM	1994	SG	CYS	129	74.577	65.903	48.312	1.00	13.14
ATOM	1995	C	CYS	129	76.403	68.661	50.637	1.00	20.64
ATOM	1996	O	CYS	129	76.886	69.624	50.046	1.00	25.40
ATOM	1997	N	VAL	130	75.929	68.807	51.888	1.00	19.35
ATOM	1998	H	VAL	130	75.382	68.086	52.274	1.00	0.00
ATOM	1999	CA	VAL	130	76.113	70.046	52.638	1.00	16.39
ATOM	2000	CB	VAL	130	75.376	69.932	53.957	1.00	18.46
ATOM	2001	CG1	VAL	130	75.660	71.129	54.845	1.00	19.50
ATOM	2002	CG2	VAL	130	73.875	69.920	53.679	1.00	19.73
ATOM	2003	C	VAL	130	77.582	70.332	52.888	1.00	17.73
ATOM	2004	O	VAL	130	78.047	71.462	52.740	1.00	20.31
ATOM	2005	N	LEU	131	78.361	69.311	53.261	1.00	17.85
ATOM	2006	H	LEU	131	77.929	68.464	53.481	1.00	0.00
ATOM	2007	CA	LEU	131	79.803	69.458	53.443	1.00	17.66
ATOM	2008	CB	LEU	131	80.352	68.199	54.164	1.00	15.83
ATOM	2009	CG	LEU	131	80.033	67.931	55.628	1.00	11.91
ATOM	2010	CD1	LEU	131	80.649	66.653	56.013	1.00	13.15
ATOM	2011	CD2	LEU	131	80.651	68.918	56.532	1.00	8.85
ATOM	2012	C	LEU	131	80.602	69.733	52.144	1.00	18.86
ATOM	2013	O	LEU	131	81.370	70.711	52.138	1.00	22.70
ATOM	2014	N	TYR	132	80.498	68.981	51.030	1.00	16.66
ATOM	2015	H	TYR	132	79.973	68.158	51.078	1.00	0.00
ATOM	2016	CA	TYR	132	81.170	69.362	49.785	1.00	16.60

FIGURE 1 (CONT.)

ATOM	2017	CB	TYR	132	80.875	68.352	48.691	1.00	19.58
ATOM	2018	CG	TYR	132	81.861	68.425	47.528	1.00	19.31
ATOM	2019	CD1	TYR	132	83.194	68.041	47.710	1.00	21.49
ATOM	2020	CE1	TYR	132	84.103	68.084	46.652	1.00	21.21
ATOM	2021	CD2	TYR	132	81.441	68.858	46.283	1.00	20.22
ATOM	2022	CE2	TYR	132	82.344	68.910	45.224	1.00	23.07
ATOM	2023	CZ	TYR	132	83.671	68.516	45.407	1.00	22.64
ATOM	2024	OH	TYR	132	84.548	68.510	44.336	1.00	21.77
ATOM	2025	HH	TYR	132	84.167	69.001	43.592	1.00	0.00
ATOM	2026	C	TYR	132	80.779	70.738	49.257	1.00	16.57
ATOM	2027	O	TYR	132	81.607	71.514	48.802	1.00	19.22
ATOM	2028	N	LEU	133	79.508	71.104	49.286	1.00	17.52
ATOM	2029	H	LEU	133	78.831	70.445	49.557	1.00	0.00
ATOM	2030	CA	LEU	133	79.096	72.425	48.883	1.00	15.66
ATOM	2031	CB	LEU	133	77.587	72.450	48.705	1.00	13.55
ATOM	2032	CG	LEU	133	77.053	71.740	47.500	1.00	10.97
ATOM	2033	CD1	LEU	133	75.537	71.824	47.453	1.00	14.01
ATOM	2034	CD2	LEU	133	77.668	72.364	46.279	1.00	10.16
ATOM	2035	C	LEU	133	79.512	73.498	49.883	1.00	18.62
ATOM	2036	O	LEU	133	79.889	74.597	49.456	1.00	19.81
ATOM	2037	N	TRP	134	79.498	73.285	51.215	1.00	18.98
ATOM	2038	H	TRP	134	79.091	72.465	51.555	1.00	0.00
ATOM	2039	CA	TRP	134	79.982	74.331	52.150	1.00	19.07
ATOM	2040	CB	TRP	134	79.616	73.874	53.572	1.00	17.38
ATOM	2041	CG	TRP	134	78.415	74.590	54.147	1.00	15.74
ATOM	2042	CD2	TRP	134	77.118	74.595	53.657	1.00	15.85
ATOM	2043	CE2	TRP	134	76.476	75.480	54.567	1.00	15.31
ATOM	2044	CE3	TRP	134	76.386	74.005	52.611	1.00	12.41
ATOM	2045	CD1	TRP	134	78.559	75.385	55.256	1.00	17.13
ATOM	2046	NE1	TRP	134	77.367	75.920	55.482	1.00	19.23
ATOM	2047	HE1	TRP	134	77.155	76.516	56.234	1.00	0.00
ATOM	2048	CZ2	TRP	134	75.121	75.775	54.442	1.00	9.40
ATOM	2049	CZ3	TRP	134	75.032	74.309	52.493	1.00	11.07
ATOM	2050	CH2	TRP	134	74.413	75.183	53.400	1.00	10.22
ATOM	2051	C	TRP	134	81.504	74.612	52.000	1.00	17.80
ATOM	2052	O	TRP	134	82.014	75.737	51.964	1.00	16.50
ATOM	2053	N	ALA	135	82.270	73.545	51.816	1.00	15.91
ATOM	2054	H	ALA	135	81.845	72.668	51.947	1.00	0.00
ATOM	2055	CA	ALA	135	83.693	73.598	51.486	1.00	16.51
ATOM	2056	CB	ALA	135	84.173	72.184	51.194	1.00	15.89
ATOM	2057	C	ALA	135	84.077	74.469	50.289	1.00	15.64
ATOM	2058	O	ALA	135	85.015	75.248	50.280	1.00	18.28
ATOM	2059	N	LEU	136	83.282	74.283	49.248	1.00	16.50
ATOM	2060	H	LEU	136	82.599	73.584	49.362	1.00	0.00
ATOM	2061	CA	LEU	136	83.361	74.901	47.938	1.00	12.85

47/145

FIGURE 1 (CONT.)

ATOM	2062	CB	LEU	136	82.445	74.108	47.021	1.00	11.26
ATOM	2063	CG	LEU	136	82.853	73.597	45.656	1.00	10.86
ATOM	2064	CD1	LEU	136	84.213	72.914	45.701	1.00	10.28
ATOM	2065	CD2	LEU	136	81.788	72.615	45.185	1.00	6.05
ATOM	2066	C	LEU	136	82.939	76.331	48.047	1.00	14.67
ATOM	2067	O	LEU	136	83.481	77.108	47.293	1.00	17.23
ATOM	2068	N	LYS	137	81.954	76.694	48.895	1.00	16.22
ATOM	2069	H	LYS	137	81.427	75.968	49.293	1.00	0.00
ATOM	2070	CA	LYS	137	81.558	78.079	49.181	1.00	12.85
ATOM	2071	CB	LYS	137	80.305	78.112	50.091	1.00	12.18
ATOM	2072	CG	LYS	137	79.813	79.510	50.506	1.00	10.11
ATOM	2073	CD	LYS	137	79.639	80.300	49.218	1.00	13.41
ATOM	2074	CE	LYS	137	79.199	81.725	49.386	1.00	16.00
ATOM	2075	NZ	LYS	137	78.815	82.254	48.091	1.00	17.45
ATOM	2076	HZ1	LYS	137	78.026	81.703	47.697	1.00	0.00
ATOM	2077	HZ2	LYS	137	79.631	82.194	47.448	1.00	0.00
ATOM	2078	HZ3	LYS	137	78.533	83.249	48.199	1.00	0.00
ATOM	2079	C	LYS	137	82.714	78.796	49.887	1.00	16.44
ATOM	2080	O	LYS	137	82.996	79.954	49.576	1.00	15.21
ATOM	2081	N	ILE	138	83.406	78.082	50.819	1.00	19.14
ATOM	2082	H	ILE	138	83.023	77.219	51.078	1.00	0.00
ATOM	2083	CA	ILE	138	84.612	78.553	51.513	1.00	18.29
ATOM	2084	CB	ILE	138	85.110	77.520	52.563	1.00	18.94
ATOM	2085	CG2	ILE	138	86.391	78.018	53.184	1.00	22.34
ATOM	2086	CG1	ILE	138	84.144	77.374	53.723	1.00	17.23
ATOM	2087	CD1	ILE	138	84.597	76.344	54.737	1.00	15.31
ATOM	2088	C	ILE	138	85.725	78.809	50.516	1.00	18.68
ATOM	2089	O	ILE	138	86.328	79.888	50.486	1.00	21.75
ATOM	2090	N	LEU	139	85.993	77.823	49.663	1.00	19.52
ATOM	2091	H	LEU	139	85.513	76.984	49.780	1.00	0.00
ATOM	2092	CA	LEU	139	86.976	77.972	48.575	1.00	20.42
ATOM	2093	CB	LEU	139	87.204	76.632	47.979	1.00	20.12
ATOM	2094	CG	LEU	139	88.472	76.350	47.222	1.00	23.85
ATOM	2095	CD1	LEU	139	89.799	76.686	47.924	1.00	19.31
ATOM	2096	CD2	LEU	139	88.368	74.879	47.014	1.00	22.70
ATOM	2097	C	LEU	139	86.638	78.972	47.452	1.00	20.73
ATOM	2098	O	LEU	139	87.469	79.786	47.016	1.00	23.33
ATOM	2099	N	TYR	140	85.394	79.029	46.986	1.00	18.86
ATOM	2100	H	TYR	140	84.748	78.426	47.387	1.00	0.00
ATOM	2101	CA	TYR	140	84.972	79.986	45.960	1.00	16.36
ATOM	2102	CB	TYR	140	84.522	79.222	44.738	1.00	10.45
ATOM	2103	CG	TYR	140	85.502	78.183	44.277	1.00	8.40
ATOM	2104	CD1	TYR	140	86.647	78.554	43.608	1.00	8.69
ATOM	2105	CE1	TYR	140	87.602	77.608	43.266	1.00	5.40
ATOM	2106	CD2	TYR	140	85.297	76.851	44.599	1.00	12.87

48/145

FIGURE 1 (CONT.)

ATOM	2107	CE2	TYR	140	86.252	75.893	44.254	1.00	12.12
ATOM	2108	CZ	TYR	140	87.395	76.296	43.590	1.00	7.67
ATOM	2109	OH	TYR	140	88.334	75.367	43.242	1.00	13.98
ATOM	2110	HH	TYR	140	89.101	75.826	42.881	1.00	0.00
ATOM	2111	C	TYR	140	83.848	80.957	46.393	1.00	17.92
ATOM	2112	O	TYR	140	82.762	80.985	45.795	1.00	19.46
ATOM	2113	N	PRO	141	84.052	81.858	47.358	1.00	18.72
ATOM	2114	CD	PRO	141	85.184	81.846	48.281	1.00	21.66
ATOM	2115	CA	PRO	141	83.082	82.812	47.871	1.00	19.26
ATOM	2116	CB	PRO	141	83.896	83.677	48.819	1.00	17.13
ATOM	2117	CG	PRO	141	84.758	82.696	49.495	1.00	18.65
ATOM	2118	C	PRO	141	82.210	83.675	46.976	1.00	20.90
ATOM	2119	O	PRO	141	81.072	84.026	47.293	1.00	18.59
ATOM	2120	N	LYS	142	82.822	84.163	45.905	1.00	24.57
ATOM	2121	H	LYS	142	83.778	83.998	45.809	1.00	0.00
ATOM	2122	CA	LYS	142	82.090	84.989	44.935	1.00	28.34
ATOM	2123	CB	LYS	142	82.819	86.293	44.636	1.00	31.54
ATOM	2124	CG	LYS	142	82.892	87.374	45.692	1.00	37.05
ATOM	2125	CD	LYS	142	84.135	87.269	46.566	1.00	42.22
ATOM	2126	CE	LYS	142	85.451	87.630	45.863	1.00	45.21
ATOM	2127	NZ	LYS	142	86.590	87.571	46.775	1.00	46.50
ATOM	2128	HZ1	LYS	142	87.459	87.787	46.244	1.00	0.00
ATOM	2129	HZ2	LYS	142	86.664	86.614	47.175	1.00	0.00
ATOM	2130	HZ3	LYS	142	86.469	88.262	47.541	1.00	0.00
ATOM	2131	C	LYS	142	81.839	84.324	43.576	1.00	29.04
ATOM	2132	O	LYS	142	81.430	84.989	42.623	1.00	32.69
ATOM	2133	N	THR	143	82.050	82.991	43.513	1.00	27.69
ATOM	2134	H	THR	143	82.216	82.562	44.377	1.00	0.00
ATOM	2135	CA	THR	143	81.988	82.134	42.309	1.00	22.07
ATOM	2136	CB	THR	143	83.303	81.352	42.140	1.00	22.81
ATOM	2137	OG1	THR	143	84.159	82.384	41.691	1.00	22.65
ATOM	2138	HG1	THR	143	85.030	82.016	41.523	1.00	0.00
ATOM	2139	CG2	THR	143	83.270	80.030	41.306	1.00	21.69
ATOM	2140	C	THR	143	80.884	81.109	42.408	1.00	22.38
ATOM	2141	O	THR	143	80.322	80.725	41.396	1.00	24.04
ATOM	2142	N	LEU	144	80.665	80.578	43.611	1.00	18.57
ATOM	2143	H	LEU	144	81.201	80.890	44.371	1.00	0.00
ATOM	2144	CA	LEU	144	79.700	79.521	43.883	1.00	19.42
ATOM	2145	CB	LEU	144	80.465	78.339	44.480	1.00	17.34
ATOM	2146	CG	LEU	144	80.157	76.889	44.858	1.00	15.74
ATOM	2147	CD1	LEU	144	79.106	76.767	45.922	1.00	16.50
ATOM	2148	CD2	LEU	144	79.799	76.186	43.630	1.00	14.36
ATOM	2149	C	LEU	144	78.662	80.075	44.865	1.00	20.27
ATOM	2150	O	LEU	144	78.964	80.536	45.967	1.00	20.47
ATOM	2151	N	PHE	145	77.394	80.069	44.476	1.00	19.18

49/145

FIGURE 1 (CONT.)

ATOM	2152	H	PHE	145	77.179	79.753	43.573	1.00	0.00
ATOM	2153	CA	PHE	145	76.347	80.604	45.333	1.00	17.36
ATOM	2154	CB	PHE	145	75.652	81.766	44.676	1.00	15.43
ATOM	2155	CG	PHE	145	76.631	82.861	44.297	1.00	20.91
ATOM	2156	CD1	PHE	145	77.256	82.852	43.028	1.00	19.52
ATOM	2157	CD2	PHE	145	76.896	83.891	45.217	1.00	19.96
ATOM	2158	CE1	PHE	145	78.137	83.886	42.693	1.00	18.11
ATOM	2159	CE2	PHE	145	77.780	84.912	44.858	1.00	17.57
ATOM	2160	CZ	PHE	145	78.391	84.908	43.604	1.00	17.39
ATOM	2161	C	PHE	145	75.303	79.574	45.670	1.00	16.04
ATOM	2162	O	PHE	145	74.794	78.879	44.814	1.00	17.70
ATOM	2163	N	LEU	146	74.977	79.450	46.936	1.00	16.74
ATOM	2164	H	LEU	146	75.452	80.015	47.579	1.00	0.00
ATOM	2165	CA	LEU	146	73.952	78.546	47.416	1.00	12.62
ATOM	2166	CB	LEU	146	74.526	77.711	48.529	1.00	11.21
ATOM	2167	CG	LEU	146	75.825	77.017	48.194	1.00	9.46
ATOM	2168	CD1	LEU	146	76.429	76.471	49.453	1.00	11.74
ATOM	2169	CD2	LEU	146	75.572	75.948	47.175	1.00	8.82
ATOM	2170	C	LEU	146	72.780	79.348	47.918	1.00	13.23
ATOM	2171	O	LEU	146	72.948	80.294	48.672	1.00	15.41
ATOM	2172	N	LEU	147	71.575	79.035	47.472	1.00	17.20
ATOM	2173	H	LEU	147	71.527	78.312	46.813	1.00	0.00
ATOM	2174	CA	LEU	147	70.329	79.684	47.922	1.00	17.47
ATOM	2175	CB	LEU	147	69.396	79.876	46.756	1.00	15.96
ATOM	2176	CG	LEU	147	69.100	81.254	46.284	1.00	12.11
ATOM	2177	CD1	LEU	147	70.306	81.993	45.808	1.00	8.16
ATOM	2178	CD2	LEU	147	68.107	81.073	45.159	1.00	16.92
ATOM	2179	C	LEU	147	69.591	78.830	48.951	1.00	18.76
ATOM	2180	O	LEU	147	69.905	77.624	49.097	1.00	18.35
ATOM	2181	N	ARG	148	68.597	79.369	49.669	1.00	16.91
ATOM	2182	H	ARG	148	68.381	80.321	49.588	1.00	0.00
ATOM	2183	CA	ARG	148	67.854	78.482	50.562	1.00	16.55
ATOM	2184	CB	ARG	148	67.310	79.262	51.761	1.00	17.09
ATOM	2185	CG	ARG	148	66.916	78.326	52.915	1.00	12.47
ATOM	2186	CD	ARG	148	66.540	79.161	54.092	1.00	14.01
ATOM	2187	NE	ARG	148	66.324	78.285	55.214	1.00	16.19
ATOM	2188	HE	ARG	148	66.261	77.327	55.042	1.00	0.00
ATOM	2189	CZ	ARG	148	66.170	78.755	56.460	1.00	18.74
ATOM	2190	NH1	ARG	148	66.047	77.913	57.488	1.00	15.67
ATOM	2191	HH11	ARG	148	66.061	76.927	57.327	1.00	0.00
ATOM	2192	HH12	ARG	148	65.927	78.271	58.413	1.00	0.00
ATOM	2193	NH2	ARG	148	66.091	80.054	56.712	1.00	18.45
ATOM	2194	HH21	ARG	148	66.131	80.719	55.969	1.00	0.00
ATOM	2195	HH22	ARG	148	66.005	80.369	57.654	1.00	0.00
ATOM	2196	C	ARG	148	66.690	77.716	49.921	1.00	17.74

FIGURE 1 (CONT.)

ATOM	2197	O	ARG	148	65.989	78.189	49.001	1.00	21.65
ATOM	2198	N	GLY	149	66.441	76.480	50.366	1.00	16.77
ATOM	2199	H	GLY	149	66.929	76.204	51.167	1.00	0.00
ATOM	2200	CA	GLY	149	65.327	75.708	49.820	1.00	15.53
ATOM	2201	C	GLY	149	64.263	75.417	50.851	1.00	15.88
ATOM	2202	O	GLY	149	64.584	75.466	52.018	1.00	16.06
ATOM	2203	N	ASN	150	63.005	75.090	50.551	1.00	18.25
ATOM	2204	H	ASN	150	62.665	75.330	49.670	1.00	0.00
ATOM	2205	CA	ASN	150	62.032	74.694	51.592	1.00	17.64
ATOM	2206	CB	ASN	150	60.718	74.270	50.931	1.00	15.57
ATOM	2207	CG	ASN	150	60.692	73.038	50.052	1.00	18.41
ATOM	2208	OD1	ASN	150	61.490	72.851	49.134	1.00	22.57
ATOM	2209	ND2	ASN	150	59.779	72.108	50.190	1.00	16.22
ATOM	2210	HD21	ASN	150	59.824	71.334	49.615	1.00	0.00
ATOM	2211	HD22	ASN	150	59.079	72.262	50.854	1.00	0.00
ATOM	2212	C	ASN	150	62.425	73.602	52.591	1.00	16.35
ATOM	2213	O	ASN	150	61.888	73.465	53.685	1.00	19.15
ATOM	2214	N	HIS	151	63.360	72.769	52.164	1.00	15.59
ATOM	2215	H	HIS	151	63.664	72.932	51.258	1.00	0.00
ATOM	2216	CA	HIS	151	63.925	71.686	52.956	1.00	16.17
ATOM	2217	CB	HIS	151	64.388	70.529	52.050	1.00	16.86
ATOM	2218	CG	HIS	151	63.324	69.501	51.694	1.00	17.72
ATOM	2219	CD2	HIS	151	62.205	69.659	50.926	1.00	13.32
ATOM	2220	ND1	HIS	151	63.300	68.256	52.154	1.00	18.26
ATOM	2221	HD1	HIS	151	63.992	67.852	52.701	1.00	0.00
ATOM	2222	CE1	HIS	151	62.248	67.645	51.733	1.00	13.78
ATOM	2223	NE2	HIS	151	61.605	68.496	51.000	1.00	15.60
ATOM	2224	HE2	HIS	151	60.718	68.268	50.657	1.00	0.00
ATOM	2225	C	HIS	151	65.116	72.104	53.805	1.00	16.72
ATOM	2226	O	HIS	151	65.557	71.342	54.662	1.00	20.69
ATOM	2227	N	GLU	152	65.717	73.268	53.614	1.00	15.30
ATOM	2228	H	GLU	152	65.303	73.948	53.048	1.00	0.00
ATOM	2229	CA	GLU	152	66.848	73.639	54.444	1.00	15.12
ATOM	2230	CB	GLU	152	67.780	74.546	53.689	1.00	16.74
ATOM	2231	CG	GLU	152	68.821	73.773	52.906	1.00	16.17
ATOM	2232	CD	GLU	152	68.303	73.183	51.618	1.00	18.12
ATOM	2233	OE1	GLU	152	68.307	71.966	51.480	1.00	19.15
ATOM	2234	OE2	GLU	152	67.893	73.952	50.760	1.00	18.61
ATOM	2235	C	GLU	152	66.325	74.352	55.666	1.00	15.54
ATOM	2236	O	GLU	152	66.391	75.559	55.844	1.00	16.27
ATOM	2237	N	CYS	153	65.688	73.565	56.504	1.00	15.65
ATOM	2238	H	CYS	153	65.705	72.595	56.336	1.00	0.00
ATOM	2239	CA	CYS	153	65.046	74.081	57.688	1.00	15.82
ATOM	2240	CB	CYS	153	63.668	74.671	57.312	1.00	15.39
ATOM	2241	SG	CYS	153	62.287	73.536	56.957	1.00	21.31

51/145

FIGURE 1 (CONT.)

ATOM	2242	C	CYS	153	64.888	72.935	58.683	1.00	17.91
ATOM	2243	O	CYS	153	65.071	71.776	58.329	1.00	16.43
ATOM	2244	N	ARG	154	64.561	73.238	59.952	1.00	21.58
ATOM	2245	H	ARG	154	64.686	74.176	60.179	1.00	0.00
ATOM	2246	CA	ARG	154	64.279	72.262	61.028	1.00	19.93
ATOM	2247	CB	ARG	154	64.084	72.966	62.357	1.00	19.03
ATOM	2248	CG	ARG	154	65.308	73.852	62.627	1.00	20.60
ATOM	2249	CD	ARG	154	65.257	74.687	63.891	1.00	17.76
ATOM	2250	NE	ARG	154	66.423	75.541	63.914	1.00	16.58
ATOM	2251	HE	ARG	154	67.189	75.287	64.470	1.00	0.00
ATOM	2252	CZ	ARG	154	66.505	76.662	63.175	1.00	19.09
ATOM	2253	NH1	ARG	154	67.610	77.373	63.253	1.00	18.69
ATOM	2254	HH11	ARG	154	67.691	78.209	62.731	1.00	0.00
ATOM	2255	HH12	ARG	154	68.357	77.073	63.846	1.00	0.00
ATOM	2256	NH2	ARG	154	65.543	77.115	62.356	1.00	18.35
ATOM	2257	HH21	ARG	154	64.683	76.615	62.272	1.00	0.00
ATOM	2258	HH22	ARG	154	65.679	77.969	61.856	1.00	0.00
ATOM	2259	C	ARG	154	63.063	71.397	60.814	1.00	20.36
ATOM	2260	O	ARG	154	63.123	70.174	60.771	1.00	20.75
ATOM	2261	N	HIS	155	61.908	72.014	60.597	1.00	22.57
ATOM	2262	H	HIS	155	61.899	72.985	60.673	1.00	0.00
ATOM	2263	CA	HIS	155	60.669	71.239	60.407	1.00	22.82
ATOM	2264	CB	HIS	155	59.487	72.150	60.058	1.00	29.04
ATOM	2265	CG	HIS	155	59.315	72.799	58.665	1.00	39.10
ATOM	2266	CD2	HIS	155	59.857	74.025	58.281	1.00	43.42
ATOM	2267	ND1	HIS	155	58.555	72.402	57.630	1.00	42.46
ATOM	2268	HD1	HIS	155	57.946	71.632	57.595	1.00	0.00
ATOM	2269	CE1	HIS	155	58.629	73.331	56.681	1.00	47.02
ATOM	2270	NE2	HIS	155	59.419	74.306	57.080	1.00	44.98
ATOM	2271	HE2	HIS	155	59.592	75.130	56.580	1.00	0.00
ATOM	2272	C	HIS	155	60.688	70.139	59.372	1.00	20.10
ATOM	2273	O	HIS	155	60.095	69.100	59.624	1.00	19.75
ATOM	2274	N	LEU	156	61.349	70.325	58.225	1.00	17.62
ATOM	2275	H	LEU	156	61.959	71.079	58.115	1.00	0.00
ATOM	2276	CA	LEU	156	61.325	69.268	57.246	1.00	17.78
ATOM	2277	CB	LEU	156	61.421	69.850	55.841	1.00	17.76
ATOM	2278	CG	LEU	156	60.160	70.501	55.256	1.00	19.31
ATOM	2279	CD1	LEU	156	60.301	70.648	53.753	1.00	19.31
ATOM	2280	CD2	LEU	156	58.938	69.612	55.471	1.00	20.01
ATOM	2281	C	LEU	156	62.396	68.184	57.410	1.00	20.32
ATOM	2282	O	LEU	156	62.165	67.016	57.069	1.00	19.81
ATOM	2283	N	THR	157	63.555	68.537	57.964	1.00	19.67
ATOM	2284	H	THR	157	63.698	69.464	58.247	1.00	0.00
ATOM	2285	CA	THR	157	64.658	67.616	58.209	1.00	18.19
ATOM	2286	CB	THR	157	65.948	68.424	58.305	1.00	19.00

52/145

FIGURE 1 (CONT.)

ATOM	2287	OG1	THR	157	65.694	69.404	59.299	1.00	20.10
ATOM	2288	HG1	THR	157	66.504	69.705	59.728	1.00	0.00
ATOM	2289	CG2	THR	157	66.359	69.095	56.982	1.00	16.35
ATOM	2290	C	THR	157	64.456	66.770	59.453	1.00	17.89
ATOM	2291	O	THR	157	64.950	65.638	59.536	1.00	22.22
ATOM	2292	N	ALA	158	63.770	67.262	60.464	1.00	18.27
ATOM	2293	H	ALA	158	63.693	68.242	60.521	1.00	0.00
ATOM	2294	CA	ALA	158	63.265	66.388	61.534	1.00	20.15
ATOM	2295	CB	ALA	158	62.508	67.184	62.614	1.00	20.41
ATOM	2296	C	ALA	158	62.284	65.310	61.030	1.00	21.54
ATOM	2297	O	ALA	158	62.366	64.138	61.369	1.00	22.99
ATOM	2298	N	TYR	159	61.324	65.721	60.198	1.00	23.26
ATOM	2299	H	TYR	159	61.305	66.679	60.004	1.00	0.00
ATOM	2300	CA	TYR	159	60.319	64.856	59.611	1.00	22.59
ATOM	2301	CB	TYR	159	59.238	65.782	59.161	1.00	24.56
ATOM	2302	CG	TYR	159	58.184	65.233	58.212	1.00	31.97
ATOM	2303	CD1	TYR	159	57.414	64.088	58.495	1.00	33.28
ATOM	2304	CE1	TYR	159	56.472	63.646	57.563	1.00	33.66
ATOM	2305	CD2	TYR	159	57.999	65.922	57.006	1.00	34.83
ATOM	2306	CE2	TYR	159	57.063	65.481	56.084	1.00	35.68
ATOM	2307	CZ	TYR	159	56.309	64.351	56.371	1.00	36.53
ATOM	2308	OH	TYR	159	55.356	63.963	55.436	1.00	43.54
ATOM	2309	HH	TYR	159	55.344	64.594	54.709	1.00	0.00
ATOM	2310	C	TYR	159	60.795	63.937	58.505	1.00	22.41
ATOM	2311	O	TYR	159	60.403	62.774	58.414	1.00	26.10
ATOM	2312	N	PHE	160	61.603	64.416	57.595	1.00	21.57
ATOM	2313	H	PHE	160	61.829	65.351	57.659	1.00	0.00
ATOM	2314	CA	PHE	160	62.165	63.538	56.585	1.00	21.14
ATOM	2315	CB	PHE	160	62.495	64.318	55.375	1.00	20.94
ATOM	2316	CG	PHE	160	61.285	64.525	54.519	1.00	16.06
ATOM	2317	CD1	PHE	160	60.636	65.751	54.580	1.00	14.80
ATOM	2318	CD2	PHE	160	60.876	63.498	53.683	1.00	12.54
ATOM	2319	CE1	PHE	160	59.542	65.955	53.769	1.00	11.64
ATOM	2320	CE2	PHE	160	59.775	63.727	52.880	1.00	15.40
ATOM	2321	CZ	PHE	160	59.116	64.956	52.926	1.00	14.17
ATOM	2322	C	PHE	160	63.392	62.762	56.994	1.00	22.48
ATOM	2323	O	PHE	160	63.292	62.052	57.989	1.00	27.43
ATOM	2324	N	THR	161	64.541	62.737	56.304	1.00	22.40
ATOM	2325	H	THR	161	64.555	62.989	55.363	1.00	0.00
ATOM	2326	CA	THR	161	65.678	61.980	56.837	1.00	20.17
ATOM	2327	CB	THR	161	66.190	60.926	55.800	1.00	20.42
ATOM	2328	OG1	THR	161	66.043	61.425	54.469	1.00	24.05
ATOM	2329	HG1	THR	161	66.128	60.659	53.882	1.00	0.00
ATOM	2330	CG2	THR	161	65.434	59.629	55.980	1.00	19.93
ATOM	2331	C	THR	161	66.909	62.698	57.363	1.00	19.02

53/145

FIGURE 1 (CONT.)

ATOM	2332	O	THR	161	67.738	62.067	58.011	1.00	20.03
ATOM	2333	N	PHE	162	67.126	64.001	57.256	1.00	19.02
ATOM	2334	H	PHE	162	66.378	64.563	56.987	1.00	0.00
ATOM	2335	CA	PHE	162	68.425	64.587	57.627	1.00	17.61
ATOM	2336	CB	PHE	162	68.442	65.987	56.976	1.00	14.66
ATOM	2337	CG	PHE	162	69.748	66.734	57.037	1.00	11.35
ATOM	2338	CD1	PHE	162	69.748	68.035	57.548	1.00	13.12
ATOM	2339	CD2	PHE	162	70.934	66.129	56.586	1.00	13.59
ATOM	2340	CE1	PHE	162	70.946	68.750	57.613	1.00	15.89
ATOM	2341	CE2	PHE	162	72.139	66.839	56.644	1.00	12.23
ATOM	2342	CZ	PHE	162	72.137	68.144	57.156	1.00	17.84
ATOM	2343	C	PHE	162	68.793	64.613	59.138	1.00	18.83
ATOM	2344	O	PHE	162	69.971	64.446	59.456	1.00	19.27
ATOM	2345	N	LYS	163	67.882	64.792	60.119	1.00	18.70
ATOM	2346	H	LYS	163	66.970	65.047	59.854	1.00	0.00
ATOM	2347	CA	LYS	163	68.190	64.637	61.542	1.00	16.82
ATOM	2348	CB	LYS	163	66.944	64.677	62.377	1.00	17.58
ATOM	2349	CG	LYS	163	66.609	65.881	63.245	1.00	18.14
ATOM	2350	CD	LYS	163	67.416	65.856	64.512	1.00	20.78
ATOM	2351	CE	LYS	163	66.704	66.479	65.690	1.00	19.60
ATOM	2352	NZ	LYS	163	65.758	65.520	66.204	1.00	25.18
ATOM	2353	HZ1	LYS	163	65.098	65.246	65.449	1.00	0.00
ATOM	2354	HZ2	LYS	163	65.228	65.949	66.991	1.00	0.00
ATOM	2355	HZ3	LYS	163	66.266	64.680	66.547	1.00	0.00
ATOM	2356	C	LYS	163	68.834	63.293	61.804	1.00	18.05
ATOM	2357	O	LYS	163	69.927	63.206	62.326	1.00	20.06
ATOM	2358	N	GLN	164	68.195	62.216	61.361	1.00	21.91
ATOM	2359	H	GLN	164	67.332	62.366	60.927	1.00	0.00
ATOM	2360	CA	GLN	164	68.650	60.840	61.537	1.00	22.85
ATOM	2361	CB	GLN	164	67.589	59.883	60.942	1.00	28.43
ATOM	2362	CG	GLN	164	67.854	58.355	60.879	1.00	34.39
ATOM	2363	CD	GLN	164	67.990	57.649	62.228	1.00	39.74
ATOM	2364	OE1	GLN	164	67.894	58.236	63.304	1.00	42.26
ATOM	2365	NE2	GLN	164	68.208	56.353	62.298	1.00	40.61
ATOM	2366	HE21	GLN	164	68.330	56.035	63.210	1.00	0.00
ATOM	2367	HE22	GLN	164	68.190	55.819	61.480	1.00	0.00
ATOM	2368	C	GLN	164	69.988	60.617	60.872	1.00	21.33
ATOM	2369	O	GLN	164	70.890	60.032	61.446	1.00	23.49
ATOM	2370	N	GLU	165	70.161	61.095	59.661	1.00	18.26
ATOM	2371	H	GLU	165	69.383	61.482	59.205	1.00	0.00
ATOM	2372	CA	GLU	165	71.428	61.000	58.984	1.00	17.32
ATOM	2373	CB	GLU	165	71.263	61.608	57.632	1.00	16.64
ATOM	2374	CG	GLU	165	72.401	61.201	56.770	1.00	20.06
ATOM	2375	CD	GLU	165	72.576	62.009	55.504	1.00	23.85
ATOM	2376	OE1	GLU	165	73.719	62.114	55.051	1.00	27.58

FIGURE 1 (CONT.)

ATOM	2377	OE2	GLU	165	71.593	62.503	54.958	1.00	25.48
ATOM	2378	C	GLU	165	72.525	61.716	59.786	1.00	18.81
ATOM	2379	O	GLU	165	73.508	61.084	60.176	1.00	20.10
ATOM	2380	N	CYS	166	72.434	63.019	60.090	1.00	20.20
ATOM	2381	H	CYS	166	71.666	63.522	59.743	1.00	0.00
ATOM	2382	CA	CYS	166	73.397	63.684	60.956	1.00	19.98
ATOM	2383	CB	CYS	166	72.959	65.013	61.368	1.00	19.93
ATOM	2384	SG	CYS	166	72.991	66.202	60.036	1.00	20.30
ATOM	2385	C	CYS	166	73.668	62.973	62.276	1.00	23.22
ATOM	2386	O	CYS	166	74.768	63.076	62.799	1.00	26.79
ATOM	2387	N	ALA	167	72.717	62.242	62.865	1.00	23.64
ATOM	2388	H	ALA	167	71.809	62.297	62.491	1.00	0.00
ATOM	2389	CA	ALA	167	72.924	61.487	64.103	1.00	20.08
ATOM	2390	CB	ALA	167	71.640	61.229	64.780	1.00	20.11
ATOM	2391	C	ALA	167	73.578	60.139	63.999	1.00	22.48
ATOM	2392	O	ALA	167	74.210	59.614	64.910	1.00	25.92
ATOM	2393	N	ILE	168	73.294	59.480	62.898	1.00	24.17
ATOM	2394	H	ILE	168	72.617	59.864	62.304	1.00	0.00
ATOM	2395	CA	ILE	168	73.892	58.181	62.576	1.00	22.74
ATOM	2396	CB	ILE	168	73.000	57.503	61.469	1.00	20.81
ATOM	2397	CG2	ILE	168	73.675	56.292	60.907	1.00	20.17
ATOM	2398	CG1	ILE	168	71.649	57.108	62.050	1.00	21.66
ATOM	2399	CD1	ILE	168	71.609	55.993	63.092	1.00	18.60
ATOM	2400	C	ILE	168	75.337	58.368	62.094	1.00	21.39
ATOM	2401	O	ILE	168	76.218	57.544	62.264	1.00	23.79
ATOM	2402	N	LYS	169	75.579	59.411	61.341	1.00	20.61
ATOM	2403	H	LYS	169	74.841	60.022	61.143	1.00	0.00
ATOM	2404	CA	LYS	169	76.883	59.577	60.747	1.00	20.14
ATOM	2405	CB	LYS	169	76.739	60.253	59.380	1.00	19.11
ATOM	2406	CG	LYS	169	76.205	59.281	58.350	1.00	17.14
ATOM	2407	CD	LYS	169	75.886	60.011	57.053	1.00	20.16
ATOM	2408	CE	LYS	169	75.215	59.048	56.075	1.00	18.23
ATOM	2409	NZ	LYS	169	75.288	59.560	54.725	1.00	14.06
ATOM	2410	HZ1	LYS	169	74.745	58.937	54.093	1.00	0.00
ATOM	2411	HZ2	LYS	169	76.281	59.579	54.416	1.00	0.00
ATOM	2412	HZ3	LYS	169	74.896	60.521	54.688	1.00	0.00
ATOM	2413	C	LYS	169	77.813	60.369	61.621	1.00	20.17
ATOM	2414	O	LYS	169	78.973	60.006	61.829	1.00	20.58
ATOM	2415	N	TYR	170	77.262	61.485	62.079	1.00	18.41
ATOM	2416	H	TYR	170	76.302	61.607	61.954	1.00	0.00
ATOM	2417	CA	TYR	170	78.006	62.434	62.888	1.00	20.51
ATOM	2418	CB	TYR	170	78.157	63.809	62.181	1.00	17.92
ATOM	2419	CG	TYR	170	79.151	63.774	61.026	1.00	18.40
ATOM	2420	CD1	TYR	170	78.740	63.209	59.806	1.00	16.17
ATOM	2421	CE1	TYR	170	79.615	63.131	58.744	1.00	14.27

55/145

FIGURE 1 (CONT.)

ATOM	2422	CD2	TYR	170	80.450	64.276	61.175	1.00	14.21
ATOM	2423	CE2	TYR	170	81.334	64.203	60.099	1.00	16.01
ATOM	2424	CZ	TYR	170	80.897	63.625	58.906	1.00	14.97
ATOM	2425	OH	TYR	170	81.740	63.500	57.847	1.00	17.07
ATOM	2426	HH	TYR	170	81.237	63.229	57.070	1.00	0.00
ATOM	2427	C	TYR	170	77.256	62.615	64.189	1.00	21.99
ATOM	2428	O	TYR	170	77.031	61.606	64.846	1.00	24.17
ATOM	2429	N	SER	171	76.816	63.797	64.622	1.00	20.67
ATOM	2430	H	SER	171	76.846	64.576	64.041	1.00	0.00
ATOM	2431	CA	SER	171	76.043	63.858	65.833	1.00	19.55
ATOM	2432	CB	SER	171	76.889	64.244	66.999	1.00	23.18
ATOM	2433	OG	SER	171	77.216	65.638	67.049	1.00	26.67
ATOM	2434	HG	SER	171	78.030	65.697	67.570	1.00	0.00
ATOM	2435	C	SER	171	74.984	64.891	65.696	1.00	18.96
ATOM	2436	O	SER	171	74.840	65.509	64.663	1.00	19.86
ATOM	2437	N	GLU	172	74.205	65.156	66.722	1.00	22.06
ATOM	2438	H	GLU	172	74.182	64.520	67.465	1.00	0.00
ATOM	2439	CA	GLU	172	73.269	66.273	66.705	1.00	22.05
ATOM	2440	CB	GLU	172	72.346	66.189	67.911	1.00	25.25
ATOM	2441	CG	GLU	172	70.860	66.179	67.520	1.00	32.45
ATOM	2442	CD	GLU	172	69.977	67.225	68.201	1.00	35.10
ATOM	2443	OE1	GLU	172	69.813	67.152	69.428	1.00	32.81
ATOM	2444	OE2	GLU	172	69.466	68.102	67.483	1.00	37.52
ATOM	2445	C	GLU	172	73.922	67.649	66.691	1.00	21.13
ATOM	2446	O	GLU	172	73.256	68.596	66.305	1.00	21.82
ATOM	2447	N	ALA	173	75.197	67.805	67.085	1.00	20.84
ATOM	2448	H	ALA	173	75.652	66.995	67.388	1.00	0.00
ATOM	2449	CA	ALA	173	75.947	69.095	67.093	1.00	19.33
ATOM	2450	CB	ALA	173	77.308	68.994	67.846	1.00	13.85
ATOM	2451	C	ALA	173	76.249	69.548	65.669	1.00	18.52
ATOM	2452	O	ALA	173	76.010	70.692	65.271	1.00	18.58
ATOM	2453	N	VAL	174	76.696	68.565	64.887	1.00	18.02
ATOM	2454	H	VAL	174	76.980	67.730	65.312	1.00	0.00
ATOM	2455	CA	VAL	174	76.768	68.719	63.442	1.00	18.30
ATOM	2456	CB	VAL	174	77.335	67.424	62.896	1.00	16.65
ATOM	2457	CG1	VAL	174	77.165	67.291	61.375	1.00	12.98
ATOM	2458	CG2	VAL	174	78.776	67.393	63.368	1.00	11.87
ATOM	2459	C	VAL	174	75.339	69.024	62.899	1.00	21.54
ATOM	2460	O	VAL	174	75.194	70.015	62.160	1.00	24.23
ATOM	2461	N	TYR	175	74.243	68.294	63.281	1.00	20.24
ATOM	2462	H	TYR	175	74.397	67.465	63.778	1.00	0.00
ATOM	2463	CA	TYR	175	72.854	68.655	62.865	1.00	19.96
ATOM	2464	CB	TYR	175	71.778	67.816	63.553	1.00	19.12
ATOM	2465	CG	TYR	175	70.387	68.143	63.032	1.00	18.62
ATOM	2466	CD1	TYR	175	69.999	67.772	61.728	1.00	19.51

56/145

FIGURE 1 (CONT.)

ATOM	2467	CE1	TYR	175	68.749	68.125	61.229	1.00	17.76
ATOM	2468	CD2	TYR	175	69.510	68.863	63.837	1.00	20.99
ATOM	2469	CE2	TYR	175	68.249	69.234	63.347	1.00	21.28
ATOM	2470	CZ	TYR	175	67.895	68.860	62.052	1.00	22.17
ATOM	2471	OH	TYR	175	66.675	69.258	61.595	1.00	22.72
ATOM	2472	HH	TYR	175	66.192	69.692	62.305	1.00	0.00
ATOM	2473	C	TYR	175	72.464	70.103	63.161	1.00	19.51
ATOM	2474	O	TYR	175	72.014	70.854	62.308	1.00	17.87
ATOM	2475	N	ASP	176	72.684	70.495	64.412	1.00	21.61
ATOM	2476	H	ASP	176	73.072	69.846	65.019	1.00	0.00
ATOM	2477	CA	ASP	176	72.421	71.818	64.897	1.00	21.88
ATOM	2478	CB	ASP	176	72.731	71.904	66.365	1.00	25.05
ATOM	2479	CG	ASP	176	71.789	71.097	67.260	1.00	26.36
ATOM	2480	OD1	ASP	176	70.667	70.780	66.858	1.00	26.01
ATOM	2481	OD2	ASP	176	72.201	70.784	68.378	1.00	28.93
ATOM	2482	C	ASP	176	73.212	72.861	64.183	1.00	21.38
ATOM	2483	O	ASP	176	72.659	73.901	63.830	1.00	25.24
ATOM	2484	N	ALA	177	74.475	72.578	63.910	1.00	20.58
ATOM	2485	H	ALA	177	74.854	71.759	64.278	1.00	0.00
ATOM	2486	CA	ALA	177	75.316	73.478	63.119	1.00	17.28
ATOM	2487	CB	ALA	177	76.663	72.903	62.813	1.00	19.85
ATOM	2488	C	ALA	177	74.741	73.774	61.761	1.00	16.97
ATOM	2489	O	ALA	177	74.797	74.906	61.277	1.00	20.43
ATOM	2490	N	CYS	178	74.222	72.728	61.115	1.00	16.07
ATOM	2491	H	CYS	178	74.351	71.837	61.516	1.00	0.00
ATOM	2492	CA	CYS	178	73.591	72.868	59.812	1.00	14.26
ATOM	2493	CB	CYS	178	73.156	71.576	59.198	1.00	10.05
ATOM	2494	SG	CYS	178	74.553	70.547	58.776	1.00	14.13
ATOM	2495	C	CYS	178	72.343	73.679	60.018	1.00	15.99
ATOM	2496	O	CYS	178	72.217	74.648	59.289	1.00	19.56
ATOM	2497	N	MET	179	71.438	73.434	60.983	1.00	15.56
ATOM	2498	H	MET	179	71.620	72.688	61.593	1.00	0.00
ATOM	2499	CA	MET	179	70.262	74.278	61.153	1.00	13.62
ATOM	2500	CB	MET	179	69.510	73.831	62.322	1.00	14.95
ATOM	2501	CG	MET	179	68.889	72.475	62.095	1.00	19.31
ATOM	2502	SD	MET	179	67.878	72.375	60.600	1.00	23.01
ATOM	2503	CE	MET	179	68.802	71.264	59.570	1.00	20.89
ATOM	2504	C	MET	179	70.595	75.738	61.321	1.00	13.60
ATOM	2505	O	MET	179	70.048	76.556	60.597	1.00	17.45
ATOM	2506	N	ASP	180	71.525	76.123	62.183	1.00	13.39
ATOM	2507	H	ASP	180	71.914	75.461	62.795	1.00	0.00
ATOM	2508	CA	ASP	180	71.958	77.504	62.227	1.00	15.87
ATOM	2509	CB	ASP	180	72.909	77.669	63.354	1.00	22.40
ATOM	2510	CG	ASP	180	72.408	77.291	64.756	1.00	29.22
ATOM	2511	OD1	ASP	180	71.467	76.503	64.903	1.00	31.24

57/145

FIGURE 1 (CONT.)

ATOM	2512	OD2	ASP	180	73.011	77.788	65.724	1.00	33.40
ATOM	2513	C	ASP	180	72.634	77.972	60.927	1.00	15.47
ATOM	2514	O	ASP	180	72.475	79.110	60.504	1.00	15.20
ATOM	2515	N	ALA	181	73.374	77.138	60.190	1.00	15.40
ATOM	2516	H	ALA	181	73.552	76.242	60.540	1.00	0.00
ATOM	2517	CA	ALA	181	73.979	77.556	58.924	1.00	14.75
ATOM	2518	CB	ALA	181	74.949	76.496	58.409	1.00	14.81
ATOM	2519	C	ALA	181	72.916	77.793	57.851	1.00	16.67
ATOM	2520	O	ALA	181	72.913	78.833	57.186	1.00	18.03
ATOM	2521	N	PHE	182	71.952	76.868	57.689	1.00	15.94
ATOM	2522	H	PHE	182	72.024	76.069	58.228	1.00	0.00
ATOM	2523	CA	PHE	182	70.841	76.985	56.748	1.00	13.91
ATOM	2524	CB	PHE	182	69.858	75.857	56.896	1.00	7.67
ATOM	2525	CG	PHE	182	70.364	74.532	56.401	1.00	6.40
ATOM	2526	CD1	PHE	182	71.603	74.399	55.759	1.00	8.30
ATOM	2527	CD2	PHE	182	69.587	73.409	56.620	1.00	5.59
ATOM	2528	CE1	PHE	182	72.049	73.139	55.348	1.00	5.21
ATOM	2529	CE2	PHE	182	70.040	72.161	56.205	1.00	4.65
ATOM	2530	CZ	PHE	182	71.266	72.019	55.571	1.00	2.88
ATOM	2531	C	PHE	182	70.076	78.280	56.970	1.00	16.76
ATOM	2532	O	PHE	182	69.732	78.914	55.967	1.00	19.69
ATOM	2533	N	ASP	183	69.890	78.749	58.223	1.00	16.36
ATOM	2534	H	ASP	183	70.109	78.163	58.982	1.00	0.00
ATOM	2535	CA	ASP	183	69.271	80.064	58.446	1.00	16.95
ATOM	2536	CB	ASP	183	69.171	80.452	59.910	1.00	14.53
ATOM	2537	CG	ASP	183	68.165	79.627	60.721	1.00	19.32
ATOM	2538	OD1	ASP	183	68.110	79.803	61.936	1.00	19.77
ATOM	2539	OD2	ASP	183	67.449	78.788	60.169	1.00	21.29
ATOM	2540	C	ASP	183	69.940	81.239	57.782	1.00	17.51
ATOM	2541	O	ASP	183	69.321	82.281	57.593	1.00	21.09
ATOM	2542	N	CYS	184	71.203	81.075	57.402	1.00	17.27
ATOM	2543	H	CYS	184	71.636	80.240	57.677	1.00	0.00
ATOM	2544	CA	CYS	184	71.982	82.113	56.747	1.00	15.00
ATOM	2545	CB	CYS	184	73.427	81.913	57.039	1.00	17.60
ATOM	2546	SG	CYS	184	73.773	82.127	58.792	1.00	22.33
ATOM	2547	C	CYS	184	71.852	82.203	55.256	1.00	15.72
ATOM	2548	O	CYS	184	72.213	83.194	54.632	1.00	18.31
ATOM	2549	N	LEU	185	71.371	81.139	54.625	1.00	16.98
ATOM	2550	H	LEU	185	70.978	80.422	55.170	1.00	0.00
ATOM	2551	CA	LEU	185	71.292	81.068	53.170	1.00	14.37
ATOM	2552	CB	LEU	185	70.728	79.709	52.752	1.00	11.79
ATOM	2553	CG	LEU	185	71.611	78.516	52.858	1.00	10.34
ATOM	2554	CD1	LEU	185	70.806	77.255	52.720	1.00	11.25
ATOM	2555	CD2	LEU	185	72.642	78.588	51.787	1.00	9.22
ATOM	2556	C	LEU	185	70.451	82.162	52.529	1.00	16.36

FIGURE 1 (CONT.)

ATOM	2557	O	LEU	185	69.265	82.337	52.899	1.00	15.95
ATOM	2558	N	PRO	186	71.038	82.896	51.546	1.00	17.90
ATOM	2559	CD	PRO	186	72.420	82.755	51.060	1.00	17.78
ATOM	2560	CA	PRO	186	70.316	83.883	50.752	1.00	17.18
ATOM	2561	CB	PRO	186	71.310	84.321	49.721	1.00	16.47
ATOM	2562	CG	PRO	186	72.655	84.078	50.366	1.00	16.90
ATOM	2563	C	PRO	186	69.042	83.287	50.169	1.00	20.05
ATOM	2564	O	PRO	186	68.949	82.110	49.771	1.00	23.20
ATOM	2565	N	LEU	187	67.983	84.069	50.251	1.00	21.80
ATOM	2566	H	LEU	187	68.079	84.938	50.688	1.00	0.00
ATOM	2567	CA	LEU	187	66.696	83.643	49.724	1.00	20.95
ATOM	2568	CB	LEU	187	65.603	84.518	50.361	1.00	24.13
ATOM	2569	CG	LEU	187	64.891	84.186	51.682	1.00	24.19
ATOM	2570	CD1	LEU	187	65.625	83.116	52.454	1.00	24.21
ATOM	2571	CD2	LEU	187	64.758	85.487	52.482	1.00	23.19
ATOM	2572	C	LEU	187	66.622	83.725	48.199	1.00	20.81
ATOM	2573	O	LEU	187	65.910	82.934	47.581	1.00	20.82
ATOM	2574	N	ALA	188	67.369	84.633	47.551	1.00	20.12
ATOM	2575	H	ALA	188	68.006	85.168	48.064	1.00	0.00
ATOM	2576	CA	ALA	188	67.230	84.817	46.118	1.00	18.91
ATOM	2577	CB	ALA	188	66.089	85.760	45.917	1.00	21.89
ATOM	2578	C	ALA	188	68.360	85.285	45.218	1.00	19.68
ATOM	2579	O	ALA	188	69.434	85.621	45.690	1.00	22.80
ATOM	2580	N	ALA	189	68.226	85.363	43.895	1.00	16.77
ATOM	2581	H	ALA	189	67.414	84.984	43.496	1.00	0.00
ATOM	2582	CA	ALA	189	69.282	85.924	43.070	1.00	15.19
ATOM	2583	CB	ALA	189	70.197	84.900	42.417	1.00	12.32
ATOM	2584	C	ALA	189	68.807	86.737	41.906	1.00	15.83
ATOM	2585	O	ALA	189	67.953	86.346	41.141	1.00	20.26
ATOM	2586	N	LEU	190	69.250	87.938	41.748	1.00	18.42
ATOM	2587	H	LEU	190	69.711	88.381	42.480	1.00	0.00
ATOM	2588	CA	LEU	190	68.962	88.658	40.549	1.00	20.82
ATOM	2589	CB	LEU	190	68.922	90.130	40.863	1.00	17.83
ATOM	2590	CG	LEU	190	68.110	91.038	39.986	1.00	16.50
ATOM	2591	CD1	LEU	190	68.825	92.366	40.033	1.00	15.88
ATOM	2592	CD2	LEU	190	67.990	90.566	38.559	1.00	12.51
ATOM	2593	C	LEU	190	70.131	88.283	39.632	1.00	24.32
ATOM	2594	O	LEU	190	71.289	88.671	39.811	1.00	29.21
ATOM	2595	N	MET	191	69.867	87.470	38.635	1.00	23.81
ATOM	2596	H	MET	191	68.955	87.120	38.571	1.00	0.00
ATOM	2597	CA	MET	191	70.902	87.026	37.745	1.00	22.55
ATOM	2598	CB	MET	191	70.620	85.577	37.551	1.00	20.51
ATOM	2599	CG	MET	191	71.842	84.811	37.195	1.00	21.57
ATOM	2600	SD	MET	191	72.150	84.928	35.435	1.00	19.85
ATOM	2601	CE	MET	191	71.021	83.700	34.864	1.00	24.25

59/145

FIGURE 1 (CONT.)

ATOM	2602	C	MET	191	70.922	87.837	36.437	1.00	24.68
ATOM	2603	O	MET	191	69.899	88.103	35.795	1.00	23.90
ATOM	2604	N	ASN	192	72.116	88.297	36.041	1.00	25.84
ATOM	2605	H	ASN	192	72.873	87.996	36.566	1.00	0.00
ATOM	2606	CA	ASN	192	72.378	89.096	34.846	1.00	26.15
ATOM	2607	CB	ASN	192	72.389	88.139	33.686	1.00	23.49
ATOM	2608	CG	ASN	192	73.226	88.725	32.601	1.00	23.02
ATOM	2609	OD1	ASN	192	74.350	89.142	32.824	1.00	23.50
ATOM	2610	ND2	ASN	192	72.752	88.831	31.407	1.00	23.61
ATOM	2611	HD21	ASN	192	71.845	88.546	31.223	1.00	0.00
ATOM	2612	HD22	ASN	192	73.364	89.228	30.765	1.00	0.00
ATOM	2613	C	ASN	192	71.448	90.290	34.546	1.00	27.11
ATOM	2614	O	ASN	192	71.046	90.534	33.412	1.00	28.53
ATOM	2615	N	GLN	193	71.040	91.008	35.606	1.00	28.08
ATOM	2616	H	GLN	193	71.441	90.744	36.457	1.00	0.00
ATOM	2617	CA	GLN	193	70.078	92.126	35.583	1.00	25.25
ATOM	2618	CB	GLN	193	70.721	93.298	34.821	1.00	27.05
ATOM	2619	CG	GLN	193	71.887	93.935	35.551	1.00	28.60
ATOM	2620	CD	GLN	193	71.440	94.840	36.681	1.00	32.33
ATOM	2621	OE1	GLN	193	71.473	96.051	36.545	1.00	37.54
ATOM	2622	NE2	GLN	193	70.958	94.476	37.851	1.00	33.44
ATOM	2623	HE21	GLN	193	70.756	95.263	38.393	1.00	0.00
ATOM	2624	HE22	GLN	193	70.811	93.550	38.090	1.00	0.00
ATOM	2625	C	GLN	193	68.712	91.805	34.990	1.00	24.06
ATOM	2626	O	GLN	193	67.984	92.687	34.571	1.00	25.42
ATOM	2627	N	GLN	194	68.336	90.538	34.904	1.00	23.26
ATOM	2628	H	GLN	194	68.944	89.867	35.272	1.00	0.00
ATOM	2629	CA	GLN	194	67.095	90.131	34.245	1.00	24.38
ATOM	2630	CB	GLN	194	67.375	89.964	32.757	1.00	25.55
ATOM	2631	CG	GLN	194	68.398	88.925	32.373	1.00	27.74
ATOM	2632	CD	GLN	194	69.051	89.051	30.999	1.00	29.30
ATOM	2633	OE1	GLN	194	70.090	88.470	30.742	1.00	31.31
ATOM	2634	NE2	GLN	194	68.610	89.725	29.976	1.00	30.09
ATOM	2635	HE21	GLN	194	67.803	90.258	30.055	1.00	0.00
ATOM	2636	HE22	GLN	194	69.163	89.617	29.179	1.00	0.00
ATOM	2637	C	GLN	194	66.357	88.883	34.746	1.00	24.97
ATOM	2638	O	GLN	194	65.133	88.743	34.581	1.00	25.45
ATOM	2639	N	PHE	195	67.072	87.917	35.319	1.00	24.06
ATOM	2640	H	PHE	195	68.045	87.998	35.357	1.00	0.00
ATOM	2641	CA	PHE	195	66.417	86.758	35.905	1.00	23.90
ATOM	2642	CB	PHE	195	67.159	85.480	35.543	1.00	23.27
ATOM	2643	CG	PHE	195	67.257	85.215	34.040	1.00	26.61
ATOM	2644	CD1	PHE	195	68.378	85.648	33.319	1.00	26.80
ATOM	2645	CD2	PHE	195	66.232	84.545	33.368	1.00	23.84
ATOM	2646	CE1	PHE	195	68.450	85.411	31.948	1.00	26.45

60/145

FIGURE 1 (CONT.)

ATOM	2647	CE2	PHE	195	66.328	84.317	32.001	1.00	22.01
ATOM	2648	CZ	PHE	195	67.430	84.748	31.286	1.00	22.08
ATOM	2649	C	PHE	195	66.310	86.836	37.429	1.00	24.12
ATOM	2650	O	PHE	195	67.161	87.383	38.120	1.00	22.90
ATOM	2651	N	LEU	196	65.214	86.315	37.966	1.00	24.31
ATOM	2652	H	LEU	196	64.509	86.011	37.353	1.00	0.00
ATOM	2653	CA	LEU	196	64.986	86.237	39.399	1.00	21.88
ATOM	2654	CB	LEU	196	63.619	86.835	39.755	1.00	20.37
ATOM	2655	CG	LEU	196	63.157	87.218	41.181	1.00	21.79
ATOM	2656	CD1	LEU	196	62.123	86.224	41.718	1.00	20.60
ATOM	2657	CD2	LEU	196	64.380	87.343	42.062	1.00	20.97
ATOM	2658	C	LEU	196	65.016	84.752	39.670	1.00	21.57
ATOM	2659	O	LEU	196	64.315	83.941	39.052	1.00	22.21
ATOM	2660	N	CYS	197	65.957	84.393	40.519	1.00	19.86
ATOM	2661	H	CYS	197	66.563	85.087	40.848	1.00	0.00
ATOM	2662	CA	CYS	197	66.125	83.006	40.873	1.00	16.44
ATOM	2663	CB	CYS	197	67.525	82.555	40.648	1.00	16.78
ATOM	2664	SG	CYS	197	68.106	83.189	39.063	1.00	17.73
ATOM	2665	C	CYS	197	65.771	82.772	42.310	1.00	14.33
ATOM	2666	O	CYS	197	66.142	83.512	43.209	1.00	13.81
ATOM	2667	N	VAL	198	64.856	81.825	42.419	1.00	13.80
ATOM	2668	H	VAL	198	64.558	81.381	41.591	1.00	0.00
ATOM	2669	CA	VAL	198	64.311	81.377	43.688	1.00	12.53
ATOM	2670	CB	VAL	198	62.930	82.082	44.089	1.00	12.56
ATOM	2671	CG1	VAL	198	63.222	83.447	44.758	1.00	6.32
ATOM	2672	CG2	VAL	198	62.011	82.238	42.873	1.00	9.16
ATOM	2673	C	VAL	198	64.075	79.885	43.667	1.00	11.58
ATOM	2674	O	VAL	198	64.195	79.216	42.645	1.00	13.15
ATOM	2675	N	HIS	199	63.784	79.329	44.830	1.00	12.16
ATOM	2676	H	HIS	199	63.831	79.909	45.619	1.00	0.00
ATOM	2677	CA	HIS	199	63.508	77.907	44.927	1.00	12.11
ATOM	2678	CB	HIS	199	63.746	77.456	46.348	1.00	11.51
ATOM	2679	CG	HIS	199	63.590	75.964	46.421	1.00	8.02
ATOM	2680	CD2	HIS	199	62.584	75.312	47.061	1.00	11.48
ATOM	2681	ND1	HIS	199	64.347	75.040	45.870	1.00	9.86
ATOM	2682	HD1	HIS	199	65.154	75.201	45.328	1.00	0.00
ATOM	2683	CE1	HIS	199	63.857	73.864	46.142	1.00	9.07
ATOM	2684	NE2	HIS	199	62.785	74.028	46.867	1.00	10.14
ATOM	2685	HE2	HIS	199	62.352	73.333	47.407	1.00	0.00
ATOM	2686	C	HIS	199	62.084	77.535	44.514	1.00	13.91
ATOM	2687	O	HIS	199	61.940	76.582	43.762	1.00	15.34
ATOM	2688	N	GLY	200	61.045	78.148	45.112	1.00	13.57
ATOM	2689	H	GLY	200	61.231	78.833	45.787	1.00	0.00
ATOM	2690	CA	GLY	200	59.656	77.933	44.742	1.00	11.83
ATOM	2691	C	GLY	200	59.100	79.049	43.858	1.00	13.43

FIGURE 1 (CONT.)

ATOM	2692	O	GLY	200	58.607	78.814	42.755	1.00	16.49
ATOM	2693	N	GLY	201	59.159	80.310	44.238	1.00	11.90
ATOM	2694	H	GLY	201	59.468	80.541	45.136	1.00	0.00
ATOM	2695	CA	GLY	201	58.685	81.311	43.333	1.00	12.38
ATOM	2696	C	GLY	201	58.161	82.571	43.979	1.00	16.15
ATOM	2697	O	GLY	201	58.796	83.237	44.793	1.00	18.28
ATOM	2698	N	LEU	202	56.940	82.885	43.594	1.00	17.53
ATOM	2699	H	LEU	202	56.444	82.177	43.149	1.00	0.00
ATOM	2700	CA	LEU	202	56.304	84.162	43.887	1.00	19.34
ATOM	2701	CB	LEU	202	55.654	84.590	42.512	1.00	17.80
ATOM	2702	CG	LEU	202	56.539	85.360	41.468	1.00	18.73
ATOM	2703	CD1	LEU	202	57.662	84.508	40.989	1.00	20.27
ATOM	2704	CD2	LEU	202	55.788	85.686	40.207	1.00	14.12
ATOM	2705	C	LEU	202	55.333	84.218	45.098	1.00	19.75
ATOM	2706	O	LEU	202	54.912	83.219	45.702	1.00	21.48
ATOM	2707	N	SER	203	54.910	85.400	45.505	1.00	20.41
ATOM	2708	H	SER	203	55.140	86.188	44.968	1.00	0.00
ATOM	2709	CA	SER	203	54.106	85.583	46.718	1.00	22.47
ATOM	2710	CB	SER	203	55.018	85.912	47.916	1.00	20.84
ATOM	2711	OG	SER	203	54.307	86.081	49.136	1.00	21.85
ATOM	2712	HG	SER	203	54.862	85.699	49.823	1.00	0.00
ATOM	2713	C	SER	203	53.121	86.732	46.525	1.00	24.74
ATOM	2714	O	SER	203	53.504	87.652	45.790	1.00	26.97
ATOM	2715	N	PRO	204	51.887	86.822	47.067	1.00	23.67
ATOM	2716	CD	PRO	204	51.058	85.718	47.485	1.00	23.37
ATOM	2717	CA	PRO	204	51.126	88.055	47.104	1.00	23.44
ATOM	2718	CB	PRO	204	49.810	87.626	47.644	1.00	22.65
ATOM	2719	CG	PRO	204	50.093	86.396	48.429	1.00	23.05
ATOM	2720	C	PRO	204	51.758	89.185	47.889	1.00	24.01
ATOM	2721	O	PRO	204	51.617	90.354	47.565	1.00	26.26
ATOM	2722	N	GLU	205	52.536	88.829	48.897	1.00	26.00
ATOM	2723	H	GLU	205	52.673	87.874	49.051	1.00	0.00
ATOM	2724	CA	GLU	205	53.186	89.783	49.803	1.00	28.20
ATOM	2725	CB	GLU	205	53.245	89.119	51.248	1.00	31.62
ATOM	2726	CG	GLU	205	51.889	88.642	51.897	1.00	39.48
ATOM	2727	CD	GLU	205	51.852	87.383	52.819	1.00	44.65
ATOM	2728	OE1	GLU	205	51.606	86.251	52.355	1.00	44.45
ATOM	2729	OE2	GLU	205	52.029	87.532	54.035	1.00	47.68
ATOM	2730	C	GLU	205	54.582	90.206	49.314	1.00	26.73
ATOM	2731	O	GLU	205	55.392	90.767	50.062	1.00	26.50
ATOM	2732	N	ILE	206	54.922	89.854	48.060	1.00	26.28
ATOM	2733	H	ILE	206	54.251	89.382	47.530	1.00	0.00
ATOM	2734	CA	ILE	206	56.200	90.195	47.380	1.00	25.36
ATOM	2735	CB	ILE	206	57.145	88.975	47.033	1.00	25.09
ATOM	2736	CG2	ILE	206	58.262	89.412	46.046	1.00	22.88

FIGURE 1 (CONT.)

ATOM	2737	CG1	ILE	206	57.743	88.381	48.318	1.00	24.84
ATOM	2738	CD1	ILE	206	58.787	89.268	49.016	1.00	27.83
ATOM	2739	C	ILE	206	55.814	90.799	46.038	1.00	24.48
ATOM	2740	O	ILE	206	55.275	90.098	45.197	1.00	27.02
ATOM	2741	N	ASN	207	56.022	92.071	45.779	1.00	23.24
ATOM	2742	H	ASN	207	56.283	92.641	46.529	1.00	0.00
ATOM	2743	CA	ASN	207	55.650	92.627	44.490	1.00	24.47
ATOM	2744	CB	ASN	207	54.504	93.611	44.678	1.00	26.63
ATOM	2745	CG	ASN	207	53.357	93.007	45.487	1.00	29.48
ATOM	2746	OD1	ASN	207	53.050	93.485	46.566	1.00	32.06
ATOM	2747	ND2	ASN	207	52.700	91.908	45.178	1.00	31.61
ATOM	2748	HD21	ASN	207	52.925	91.388	44.386	1.00	0.00
ATOM	2749	HD22	ASN	207	52.033	91.667	45.856	1.00	0.00
ATOM	2750	C	ASN	207	56.778	93.321	43.746	1.00	25.50
ATOM	2751	O	ASN	207	56.651	93.782	42.619	1.00	27.51
ATOM	2752	N	THR	208	57.917	93.422	44.414	1.00	26.73
ATOM	2753	H	THR	208	57.937	93.072	45.325	1.00	0.00
ATOM	2754	CA	THR	208	59.151	94.014	43.900	1.00	25.53
ATOM	2755	CB	THR	208	59.272	95.516	44.146	1.00	22.39
ATOM	2756	OG1	THR	208	59.117	95.672	45.540	1.00	23.21
ATOM	2757	HG1	THR	208	59.020	96.611	45.749	1.00	0.00
ATOM	2758	CG2	THR	208	58.281	96.361	43.396	1.00	20.63
ATOM	2759	C	THR	208	60.390	93.404	44.569	1.00	27.22
ATOM	2760	O	THR	208	60.326	92.879	45.683	1.00	27.04
ATOM	2761	N	LEU	209	61.552	93.445	43.924	1.00	29.14
ATOM	2762	H	LEU	209	61.520	93.760	42.993	1.00	0.00
ATOM	2763	CA	LEU	209	62.816	92.957	44.510	1.00	30.68
ATOM	2764	CB	LEU	209	63.963	93.126	43.474	1.00	29.45
ATOM	2765	CG	LEU	209	64.186	92.060	42.366	1.00	24.80
ATOM	2766	CD1	LEU	209	62.887	91.580	41.804	1.00	25.15
ATOM	2767	CD2	LEU	209	64.992	92.659	41.253	1.00	21.37
ATOM	2768	C	LEU	209	63.208	93.631	45.832	1.00	32.55
ATOM	2769	O	LEU	209	63.651	92.907	46.731	1.00	33.17
ATOM	2770	N	ASP	210	62.979	94.965	46.048	1.00	35.21
ATOM	2771	H	ASP	210	62.670	95.494	45.288	1.00	0.00
ATOM	2772	CA	ASP	210	63.206	95.633	47.369	1.00	34.60
ATOM	2773	CB	ASP	210	62.881	97.210	47.457	1.00	36.36
ATOM	2774	CG	ASP	210	61.469	97.921	47.450	1.00	42.32
ATOM	2775	OD1	ASP	210	60.416	97.405	47.880	1.00	41.10
ATOM	2776	OD2	ASP	210	61.425	99.089	47.022	1.00	43.75
ATOM	2777	C	ASP	210	62.346	94.957	48.428	1.00	33.04
ATOM	2778	O	ASP	210	62.765	94.928	49.579	1.00	33.54
ATOM	2779	N	ASP	211	61.215	94.319	48.073	1.00	31.21
ATOM	2780	H	ASP	211	60.903	94.373	47.146	1.00	0.00
ATOM	2781	CA	ASP	211	60.403	93.578	49.050	1.00	31.60

63/145

FIGURE 1 (CONT.)

ATOM	2782	CB	ASP	211	58.997	93.259	48.490	1.00	30.78
ATOM	2783	CG	ASP	211	58.013	94.453	48.517	1.00	34.51
ATOM	2784	OD1	ASP	211	58.220	95.426	49.267	1.00	33.28
ATOM	2785	OD2	ASP	211	57.018	94.402	47.781	1.00	32.68
ATOM	2786	C	ASP	211	61.000	92.274	49.563	1.00	30.20
ATOM	2787	O	ASP	211	60.552	91.750	50.573	1.00	31.80
ATOM	2788	N	ILE	212	62.012	91.749	48.864	1.00	29.16
ATOM	2789	H	ILE	212	62.204	92.163	47.997	1.00	0.00
ATOM	2790	CA	ILE	212	62.758	90.546	49.253	1.00	27.02
ATOM	2791	CB	ILE	212	63.274	89.747	48.008	1.00	25.03
ATOM	2792	CG2	ILE	212	64.083	88.560	48.497	1.00	20.39
ATOM	2793	CG1	ILE	212	62.102	89.292	47.111	1.00	25.73
ATOM	2794	CD1	ILE	212	62.370	88.448	45.818	1.00	25.10
ATOM	2795	C	ILE	212	63.945	91.048	50.067	1.00	26.68
ATOM	2796	O	ILE	212	64.308	90.505	51.109	1.00	27.21
ATOM	2797	N	ARG	213	64.557	92.140	49.596	1.00	26.19
ATOM	2798	H	ARG	213	64.243	92.475	48.728	1.00	0.00
ATOM	2799	CA	ARG	213	65.650	92.837	50.288	1.00	25.75
ATOM	2800	CB	ARG	213	66.046	94.104	49.491	1.00	25.39
ATOM	2801	CG	ARG	213	66.630	93.747	48.125	1.00	24.29
ATOM	2802	CD	ARG	213	67.101	94.871	47.167	1.00	28.21
ATOM	2803	NE	ARG	213	68.025	94.197	46.250	1.00	33.55
ATOM	2804	HE	ARG	213	68.599	93.506	46.643	1.00	0.00
ATOM	2805	CZ	ARG	213	68.174	94.400	44.919	1.00	34.03
ATOM	2806	NH1	ARG	213	69.036	93.605	44.255	1.00	34.69
ATOM	2807	HH11	ARG	213	69.192	93.728	43.274	1.00	0.00
ATOM	2808	HH12	ARG	213	69.547	92.902	44.754	1.00	0.00
ATOM	2809	NH2	ARG	213	67.524	95.359	44.250	1.00	32.23
ATOM	2810	HH21	ARG	213	66.892	95.959	44.737	1.00	0.00
ATOM	2811	HH22	ARG	213	67.675	95.468	43.268	1.00	0.00
ATOM	2812	C	ARG	213	65.229	93.210	51.715	1.00	25.40
ATOM	2813	O	ARG	213	65.940	92.934	52.657	1.00	24.17
ATOM	2814	N	LYS	214	64.023	93.735	51.900	1.00	26.47
ATOM	2815	H	LYS	214	63.508	93.960	51.098	1.00	0.00
ATOM	2816	CA	LYS	214	63.442	94.035	53.206	1.00	27.09
ATOM	2817	CB	LYS	214	62.242	94.904	52.988	1.00	27.14
ATOM	2818	CG	LYS	214	62.526	96.195	52.256	1.00	31.38
ATOM	2819	CD	LYS	214	61.180	96.895	52.279	1.00	39.60
ATOM	2820	CE	LYS	214	60.831	97.645	51.012	1.00	43.39
ATOM	2821	NZ	LYS	214	61.716	98.774	50.801	1.00	46.41
ATOM	2822	HZ1	LYS	214	62.697	98.434	50.786	1.00	0.00
ATOM	2823	HZ2	LYS	214	61.592	99.459	51.573	1.00	0.00
ATOM	2824	HZ3	LYS	214	61.489	99.225	49.891	1.00	0.00
ATOM	2825	C	LYS	214	63.027	92.852	54.112	1.00	27.76
ATOM	2826	O	LYS	214	62.427	93.010	55.185	1.00	28.38

64/145

FIGURE 1 (CONT.)

ATOM	2827	N	LEU	215	63.307	91.606	53.756	1.00	27.45
ATOM	2828	H	LEU	215	63.773	91.445	52.915	1.00	0.00
ATOM	2829	CA	LEU	215	62.935	90.505	54.641	1.00	27.46
ATOM	2830	CB	LEU	215	62.750	89.244	53.782	1.00	26.77
ATOM	2831	CG	LEU	215	61.651	89.210	52.723	1.00	24.92
ATOM	2832	CD1	LEU	215	61.645	87.865	51.998	1.00	23.35
ATOM	2833	CD2	LEU	215	60.312	89.424	53.403	1.00	21.09
ATOM	2834	C	LEU	215	63.893	90.198	55.806	1.00	26.22
ATOM	2835	O	LEU	215	65.023	90.671	55.824	1.00	28.67
ATOM	2836	N	ASP	216	63.547	89.485	56.869	1.00	26.18
ATOM	2837	H	ASP	216	62.599	89.363	57.069	1.00	0.00
ATOM	2838	CA	ASP	216	64.581	88.980	57.781	1.00	28.21
ATOM	2839	CB	ASP	216	64.208	89.255	59.256	1.00	30.34
ATOM	2840	CG	ASP	216	65.031	88.588	60.373	1.00	32.26
ATOM	2841	OD1	ASP	216	66.155	88.098	60.194	1.00	32.70
ATOM	2842	OD2	ASP	216	64.496	88.560	61.472	1.00	35.14
ATOM	2843	C	ASP	216	64.745	87.474	57.542	1.00	27.84
ATOM	2844	O	ASP	216	63.957	86.662	58.016	1.00	28.68
ATOM	2845	N	ARG	217	65.768	87.097	56.772	1.00	25.47
ATOM	2846	H	ARG	217	66.324	87.798	56.369	1.00	0.00
ATOM	2847	CA	ARG	217	65.996	85.714	56.387	1.00	22.69
ATOM	2848	CB	ARG	217	67.015	85.769	55.233	1.00	21.21
ATOM	2849	CG	ARG	217	68.357	85.015	55.411	1.00	22.14
ATOM	2850	CD	ARG	217	69.392	85.107	54.280	1.00	17.26
ATOM	2851	NE	ARG	217	69.782	86.485	54.173	1.00	16.50
ATOM	2852	HE	ARG	217	69.081	87.166	54.133	1.00	0.00
ATOM	2853	CZ	ARG	217	71.023	86.904	54.162	1.00	13.23
ATOM	2854	NH1	ARG	217	71.181	88.217	54.123	1.00	15.32
ATOM	2855	HH11	ARG	217	70.386	88.823	54.122	1.00	0.00
ATOM	2856	HH12	ARG	217	72.101	88.610	54.140	1.00	0.00
ATOM	2857	NH2	ARG	217	72.046	86.075	54.199	1.00	10.95
ATOM	2858	HH21	ARG	217	71.889	85.089	54.236	1.00	0.00
ATOM	2859	HH22	ARG	217	72.983	86.428	54.183	1.00	0.00
ATOM	2860	C	ARG	217	66.459	84.747	57.493	1.00	23.17
ATOM	2861	O	ARG	217	66.289	83.515	57.493	1.00	23.96
ATOM	2862	N	PHE	218	67.076	85.331	58.509	1.00	22.05
ATOM	2863	H	PHE	218	67.021	86.296	58.602	1.00	0.00
ATOM	2864	CA	PHE	218	67.804	84.519	59.473	1.00	18.76
ATOM	2865	CB	PHE	218	68.859	85.369	60.148	1.00	13.93
ATOM	2866	CG	PHE	218	69.866	85.970	59.189	1.00	9.96
ATOM	2867	CD1	PHE	218	70.964	85.227	58.793	1.00	12.23
ATOM	2868	CD2	PHE	218	69.716	87.278	58.766	1.00	9.77
ATOM	2869	CE1	PHE	218	71.926	85.802	57.975	1.00	12.84
ATOM	2870	CE2	PHE	218	70.674	87.855	57.949	1.00	12.20
ATOM	2871	CZ	PHE	218	71.784	87.121	57.554	1.00	14.85

65/145

FIGURE 1 (CONT.)

ATOM	2872	C	PHE	218	66.887	83.916	60.492	1.00	19.17
ATOM	2873	O	PHE	218	66.811	84.300	61.667	1.00	20.65
ATOM	2874	N	LYS	219	66.170	82.921	60.020	1.00	17.04
ATOM	2875	H	LYS	219	66.299	82.576	59.111	1.00	0.00
ATOM	2876	CA	LYS	219	65.200	82.322	60.901	1.00	19.42
ATOM	2877	CB	LYS	219	63.938	83.254	61.107	1.00	21.35
ATOM	2878	CG	LYS	219	63.089	83.464	59.848	1.00	22.74
ATOM	2879	CD	LYS	219	61.862	84.260	60.092	1.00	23.37
ATOM	2880	CE	LYS	219	62.157	85.714	60.404	1.00	28.16
ATOM	2881	NZ	LYS	219	60.926	86.466	60.216	1.00	29.93
ATOM	2882	HZ1	LYS	219	61.112	87.480	60.365	1.00	0.00
ATOM	2883	HZ2	LYS	219	60.215	86.136	60.901	1.00	0.00
ATOM	2884	HZ3	LYS	219	60.575	86.314	59.249	1.00	0.00
ATOM	2885	C	LYS	219	64.744	81.018	60.329	1.00	18.64
ATOM	2886	O	LYS	219	65.087	80.654	59.215	1.00	22.45
ATOM	2887	N	GLU	220	64.028	80.263	61.128	1.00	18.30
ATOM	2888	H	GLU	220	63.974	80.497	62.073	1.00	0.00
ATOM	2889	CA	GLU	220	63.300	79.146	60.610	1.00	19.04
ATOM	2890	CB	GLU	220	62.788	78.344	61.763	1.00	19.96
ATOM	2891	CG	GLU	220	61.744	77.280	61.423	1.00	18.40
ATOM	2892	CD	GLU	220	62.297	76.022	60.805	1.00	20.29
ATOM	2893	OE1	GLU	220	61.500	75.241	60.320	1.00	25.99
ATOM	2894	OE2	GLU	220	63.494	75.794	60.811	1.00	21.68
ATOM	2895	C	GLU	220	62.136	79.766	59.811	1.00	20.14
ATOM	2896	O	GLU	220	61.368	80.580	60.345	1.00	20.27
ATOM	2897	N	PRO	221	61.957	79.412	58.539	1.00	20.99
ATOM	2898	CD	PRO	221	62.788	78.452	57.816	1.00	19.93
ATOM	2899	CA	PRO	221	60.962	80.048	57.697	1.00	21.94
ATOM	2900	CB	PRO	221	61.192	79.392	56.330	1.00	20.46
ATOM	2901	CG	PRO	221	61.989	78.135	56.584	1.00	20.82
ATOM	2902	C	PRO	221	59.542	79.924	58.256	1.00	22.07
ATOM	2903	O	PRO	221	59.186	78.846	58.727	1.00	24.17
ATOM	2904	N	PRO	222	58.745	80.998	58.309	1.00	22.36
ATOM	2905	CD	PRO	222	59.140	82.339	57.886	1.00	25.33
ATOM	2906	CA	PRO	222	57.419	81.080	58.896	1.00	22.96
ATOM	2907	CB	PRO	222	57.068	82.511	58.841	1.00	23.67
ATOM	2908	CG	PRO	222	58.383	83.214	58.868	1.00	24.85
ATOM	2909	C	PRO	222	56.338	80.254	58.245	1.00	23.63
ATOM	2910	O	PRO	222	56.477	79.931	57.076	1.00	26.60
ATOM	2911	N	ALA	223	55.239	79.957	58.954	1.00	23.49
ATOM	2912	H	ALA	223	55.238	80.263	59.879	1.00	0.00
ATOM	2913	CA	ALA	223	54.113	79.132	58.478	1.00	21.16
ATOM	2914	CB	ALA	223	53.147	78.984	59.609	1.00	22.32
ATOM	2915	C	ALA	223	53.305	79.554	57.242	1.00	19.59
ATOM	2916	O	ALA	223	52.602	78.816	56.540	1.00	17.92

66/145

FIGURE 1 (CONT.)

ATOM	2917	N	TYR	224	53.439	80.838	57.027	1.00	16.84
ATOM	2918	H	TYR	224	54.000	81.343	57.645	1.00	0.00
ATOM	2919	CA	TYR	224	52.861	81.513	55.906	1.00	16.25
ATOM	2920	CB	TYR	224	51.418	81.811	56.204	1.00	15.17
ATOM	2921	CG	TYR	224	51.213	82.733	57.369	1.00	15.59
ATOM	2922	CD1	TYR	224	51.032	84.108	57.174	1.00	17.87
ATOM	2923	CE1	TYR	224	50.772	84.939	58.277	1.00	20.45
ATOM	2924	CD2	TYR	224	51.144	82.186	58.648	1.00	18.73
ATOM	2925	CE2	TYR	224	50.875	83.000	59.746	1.00	17.17
ATOM	2926	CZ	TYR	224	50.687	84.365	59.551	1.00	20.74
ATOM	2927	OH	TYR	224	50.371	85.146	60.639	1.00	25.58
ATOM	2928	HH	TYR	224	50.405	84.611	61.437	1.00	0.00
ATOM	2929	C	TYR	224	53.625	82.818	55.635	1.00	16.81
ATOM	2930	O	TYR	224	54.351	83.286	56.521	1.00	20.36
ATOM	2931	N	GLY	225	53.595	83.443	54.464	1.00	15.83
ATOM	2932	H	GLY	225	53.188	83.009	53.689	1.00	0.00
ATOM	2933	CA	GLY	225	54.177	84.767	54.381	1.00	17.69
ATOM	2934	C	GLY	225	55.260	84.898	53.370	1.00	19.05
ATOM	2935	O	GLY	225	55.576	83.868	52.757	1.00	20.79
ATOM	2936	N	PRO	226	55.838	86.092	53.148	1.00	20.18
ATOM	2937	CD	PRO	226	55.449	87.339	53.812	1.00	18.41
ATOM	2938	CA	PRO	226	56.791	86.347	52.041	1.00	21.78
ATOM	2939	CB	PRO	226	57.234	87.813	52.296	1.00	21.69
ATOM	2940	CG	PRO	226	56.672	88.249	53.643	1.00	19.30
ATOM	2941	C	PRO	226	57.939	85.335	51.876	1.00	23.13
ATOM	2942	O	PRO	226	58.060	84.726	50.813	1.00	26.97
ATOM	2943	N	MET	227	58.704	85.026	52.931	1.00	23.11
ATOM	2944	H	MET	227	58.602	85.615	53.706	1.00	0.00
ATOM	2945	CA	MET	227	59.742	83.966	52.984	1.00	21.70
ATOM	2946	CB	MET	227	60.527	84.058	54.301	1.00	23.84
ATOM	2947	CG	MET	227	61.365	82.882	54.788	1.00	24.76
ATOM	2948	SD	MET	227	62.278	83.431	56.225	1.00	25.43
ATOM	2949	CE	MET	227	63.668	82.354	56.244	1.00	20.64
ATOM	2950	C	MET	227	59.284	82.536	52.854	1.00	19.77
ATOM	2951	O	MET	227	59.972	81.697	52.302	1.00	22.81
ATOM	2952	N	CYS	228	58.164	82.176	53.436	1.00	22.07
ATOM	2953	H	CYS	228	57.701	82.830	53.995	1.00	0.00
ATOM	2954	CA	CYS	228	57.592	80.835	53.230	1.00	21.95
ATOM	2955	CB	CYS	228	56.257	80.703	53.936	1.00	18.38
ATOM	2956	SG	CYS	228	55.286	79.254	53.447	1.00	26.44
ATOM	2957	C	CYS	228	57.363	80.616	51.735	1.00	21.97
ATOM	2958	O	CYS	228	57.942	79.731	51.133	1.00	21.38
ATOM	2959	N	ASP	229	56.626	81.556	51.118	1.00	22.56
ATOM	2960	H	ASP	229	56.297	82.296	51.671	1.00	0.00
ATOM	2961	CA	ASP	229	56.301	81.570	49.699	1.00	21.23

67/145

FIGURE 1 (CONT.)

ATOM	2962	CB	ASP	229	55.491	82.786	49.395	1.00	21.67
ATOM	2963	CG	ASP	229	54.105	82.742	49.986	1.00	20.15
ATOM	2964	OD1	ASP	229	53.629	83.789	50.389	1.00	22.44
ATOM	2965	OD2	ASP	229	53.482	81.681	50.001	1.00	20.39
ATOM	2966	C	ASP	229	57.429	81.516	48.693	1.00	21.86
ATOM	2967	O	ASP	229	57.386	80.608	47.872	1.00	24.61
ATOM	2968	N	ILE	230	58.423	82.426	48.710	1.00	20.37
ATOM	2969	H	ILE	230	58.290	83.204	49.294	1.00	0.00
ATOM	2970	CA	ILE	230	59.663	82.334	47.913	1.00	16.29
ATOM	2971	CB	ILE	230	60.637	83.300	48.576	1.00	15.52
ATOM	2972	CG2	ILE	230	62.059	83.031	48.118	1.00	15.46
ATOM	2973	CG1	ILE	230	60.186	84.733	48.283	1.00	15.25
ATOM	2974	CD1	ILE	230	61.035	85.828	48.965	1.00	10.69
ATOM	2975	C	ILE	230	60.233	80.904	47.852	1.00	18.29
ATOM	2976	O	ILE	230	60.544	80.342	46.801	1.00	19.11
ATOM	2977	N	LEU	231	60.313	80.290	49.041	1.00	20.17
ATOM	2978	H	LEU	231	60.079	80.827	49.828	1.00	0.00
ATOM	2979	CA	LEU	231	60.752	78.923	49.291	1.00	20.25
ATOM	2980	CB	LEU	231	61.175	78.757	50.761	1.00	22.81
ATOM	2981	CG	LEU	231	62.633	78.852	51.251	1.00	22.63
ATOM	2982	CD1	LEU	231	63.391	80.037	50.704	1.00	21.65
ATOM	2983	CD2	LEU	231	62.569	79.011	52.740	1.00	22.41
ATOM	2984	C	LEU	231	59.742	77.824	48.994	1.00	21.07
ATOM	2985	O	LEU	231	60.116	76.693	48.582	1.00	18.28
ATOM	2986	N	TRP	232	58.451	78.172	49.188	1.00	20.41
ATOM	2987	H	TRP	232	58.254	79.100	49.418	1.00	0.00
ATOM	2988	CA	TRP	232	57.372	77.193	49.007	1.00	18.64
ATOM	2989	CB	TRP	232	56.488	77.151	50.216	1.00	14.75
ATOM	2990	CG	TRP	232	57.149	76.285	51.274	1.00	17.39
ATOM	2991	CD2	TRP	232	57.028	74.918	51.439	1.00	14.02
ATOM	2992	CE2	TRP	232	57.804	74.719	52.599	1.00	16.39
ATOM	2993	CE3	TRP	232	56.396	73.848	50.819	1.00	12.32
ATOM	2994	CD1	TRP	232	57.945	76.869	52.227	1.00	14.98
ATOM	2995	NE1	TRP	232	58.325	75.889	53.010	1.00	17.58
ATOM	2996	HE1	TRP	232	58.926	76.031	53.766	1.00	0.00
ATOM	2997	CZ2	TRP	232	57.959	73.461	53.177	1.00	14.24
ATOM	2998	CZ3	TRP	232	56.528	72.583	51.370	1.00	13.99
ATOM	2999	CH2	TRP	232	57.299	72.399	52.539	1.00	18.88
ATOM	3000	C	TRP	232	56.430	77.192	47.829	1.00	19.17
ATOM	3001	O	TRP	232	55.985	76.093	47.504	1.00	21.89
ATOM	3002	N	SER	233	56.150	78.272	47.101	1.00	18.92
ATOM	3003	H	SER	233	56.714	79.062	47.194	1.00	0.00
ATOM	3004	CA	SER	233	55.162	78.255	46.027	1.00	18.77
ATOM	3005	CB	SER	233	54.717	79.672	45.740	1.00	19.69
ATOM	3006	OG	SER	233	55.765	80.555	45.405	1.00	24.62

FIGURE 1 (CONT.)

ATOM	3007	HG	SER	233	55.557	81.451	45.713	1.00	0.00
ATOM	3008	C	SER	233	55.515	77.590	44.700	1.00	19.16
ATOM	3009	O	SER	233	56.643	77.212	44.411	1.00	21.40
ATOM	3010	N	ASP	234	54.472	77.286	43.952	1.00	20.13
ATOM	3011	H	ASP	234	53.600	77.580	44.291	1.00	0.00
ATOM	3012	CA	ASP	234	54.480	76.546	42.696	1.00	19.55
ATOM	3013	CB	ASP	234	53.737	75.248	42.889	1.00	20.02
ATOM	3014	CG	ASP	234	54.322	74.201	43.810	1.00	20.48
ATOM	3015	OD1	ASP	234	53.572	73.363	44.284	1.00	24.51
ATOM	3016	OD2	ASP	234	55.522	74.173	44.030	1.00	23.75
ATOM	3017	C	ASP	234	53.829	77.259	41.506	1.00	19.55
ATOM	3018	O	ASP	234	52.907	78.029	41.771	1.00	19.77
ATOM	3019	N	PRO	235	54.102	77.068	40.202	1.00	20.02
ATOM	3020	CD	PRO	235	55.153	76.224	39.616	1.00	20.95
ATOM	3021	CA	PRO	235	53.194	77.461	39.141	1.00	20.69
ATOM	3022	CB	PRO	235	53.957	77.149	37.877	1.00	18.45
ATOM	3023	CG	PRO	235	54.661	75.867	38.203	1.00	16.82
ATOM	3024	C	PRO	235	51.895	76.666	39.286	1.00	23.36
ATOM	3025	O	PRO	235	51.807	75.609	39.931	1.00	24.60
ATOM	3026	N	LEU	236	50.814	77.199	38.766	1.00	24.06
ATOM	3027	H	LEU	236	50.866	78.129	38.463	1.00	0.00
ATOM	3028	CA	LEU	236	49.548	76.475	38.708	1.00	26.52
ATOM	3029	CB	LEU	236	48.614	77.499	38.148	1.00	26.34
ATOM	3030	CG	LEU	236	47.281	77.950	38.581	1.00	21.41
ATOM	3031	CD1	LEU	236	47.148	78.407	39.983	1.00	22.30
ATOM	3032	CD2	LEU	236	47.097	79.140	37.699	1.00	23.57
ATOM	3033	C	LEU	236	49.669	75.214	37.812	1.00	28.63
ATOM	3034	O	LEU	236	50.454	75.244	36.858	1.00	31.22
ATOM	3035	N	GLU	237	48.971	74.080	37.914	1.00	30.74
ATOM	3036	H	GLU	237	48.452	73.927	38.727	1.00	0.00
ATOM	3037	CA	GLU	237	49.136	73.008	36.914	1.00	31.80
ATOM	3038	CB	GLU	237	48.343	71.787	37.345	1.00	36.38
ATOM	3039	CG	GLU	237	48.996	70.445	36.936	1.00	41.40
ATOM	3040	CD	GLU	237	48.299	69.605	35.853	1.00	42.23
ATOM	3041	OE1	GLU	237	48.970	69.170	34.905	1.00	42.11
ATOM	3042	OE2	GLU	237	47.093	69.371	35.969	1.00	45.28
ATOM	3043	C	GLU	237	48.715	73.377	35.486	1.00	31.63
ATOM	3044	O	GLU	237	48.954	72.659	34.529	1.00	32.35
ATOM	3045	N	ASP	238	48.084	74.528	35.291	1.00	32.10
ATOM	3046	H	ASP	238	47.913	75.061	36.087	1.00	0.00
ATOM	3047	CA	ASP	238	47.634	75.035	33.981	1.00	33.78
ATOM	3048	CB	ASP	238	46.088	75.066	33.926	1.00	38.61
ATOM	3049	CG	ASP	238	45.396	75.691	35.170	1.00	42.03
ATOM	3050	OD1	ASP	238	44.217	75.401	35.414	1.00	44.54
ATOM	3051	OD2	ASP	238	46.022	76.443	35.921	1.00	41.53

69/145

FIGURE 1 (CONT.)

ATOM	3052	C	ASP	238	48.176	76.448	33.769	1.00	32.06
ATOM	3053	O	ASP	238	47.462	77.438	33.712	1.00	34.74
ATOM	3054	N	PHE	239	49.470	76.653	33.754	1.00	29.17
ATOM	3055	H	PHE	239	50.048	75.876	33.897	1.00	0.00
ATOM	3056	CA	PHE	239	50.045	77.966	33.570	1.00	25.52
ATOM	3057	CB	PHE	239	51.527	77.713	33.934	1.00	24.42
ATOM	3058	CG	PHE	239	52.318	78.929	34.391	1.00	17.75
ATOM	3059	CD1	PHE	239	53.109	79.642	33.494	1.00	16.12
ATOM	3060	CD2	PHE	239	52.202	79.355	35.693	1.00	17.03
ATOM	3061	CE1	PHE	239	53.770	80.789	33.896	1.00	11.92
ATOM	3062	CE2	PHE	239	52.875	80.504	36.083	1.00	17.11
ATOM	3063	CZ	PHE	239	53.650	81.221	35.190	1.00	13.27
ATOM	3064	C	PHE	239	49.789	78.614	32.183	1.00	27.25
ATOM	3065	O	PHE	239	50.498	79.525	31.770	1.00	30.77
ATOM	3066	N	GLY	240	48.776	78.295	31.371	1.00	29.28
ATOM	3067	H	GLY	240	48.078	77.683	31.682	1.00	0.00
ATOM	3068	CA	GLY	240	48.531	78.884	30.050	1.00	25.43
ATOM	3069	C	GLY	240	47.652	77.916	29.250	1.00	28.36
ATOM	3070	O	GLY	240	46.711	77.285	29.772	1.00	28.72
ATOM	3071	CB	HIS	247	46.874	86.745	40.499	1.00	23.78
ATOM	3072	CG	HIS	247	47.488	87.811	39.579	1.00	26.72
ATOM	3073	CD2	HIS	247	48.391	88.741	40.070	1.00	26.82
ATOM	3074	ND1	HIS	247	47.287	88.174	38.292	1.00	27.63
ATOM	3075	HD1	HIS	247	46.703	87.782	37.610	1.00	0.00
ATOM	3076	CE1	HIS	247	48.005	89.252	38.017	1.00	26.96
ATOM	3077	NE2	HIS	247	48.661	89.578	39.096	1.00	26.18
ATOM	3078	HE2	HIS	247	49.292	90.330	39.148	1.00	0.00
ATOM	3079	C	HIS	247	47.588	84.374	41.031	1.00	27.00
ATOM	3080	O	HIS	247	48.406	83.588	40.593	1.00	27.40
ATOM	3081	HT1	HIS	247	45.284	83.790	39.870	1.00	0.00
ATOM	3082	HT2	HIS	247	44.643	85.276	39.581	1.00	0.00
ATOM	3083	N	HIS	247	45.362	84.792	40.159	1.00	24.65
ATOM	3084	HT3	HIS	247	44.960	84.795	41.122	1.00	0.00
ATOM	3085	CA	HIS	247	46.757	85.263	40.069	1.00	26.62
ATOM	3086	N	PHE	248	47.372	84.471	42.350	1.00	28.59
ATOM	3087	H	PHE	248	46.791	85.168	42.717	1.00	0.00
ATOM	3088	CA	PHE	248	47.942	83.598	43.398	1.00	27.05
ATOM	3089	CB	PHE	248	48.534	84.359	44.580	1.00	24.03
ATOM	3090	CG	PHE	248	49.831	84.984	44.180	1.00	19.99
ATOM	3091	CD1	PHE	248	50.926	84.152	43.972	1.00	20.39
ATOM	3092	CD2	PHE	248	49.881	86.345	43.933	1.00	17.41
ATOM	3093	CE1	PHE	248	52.095	84.717	43.488	1.00	19.09
ATOM	3094	CE2	PHE	248	51.055	86.895	43.454	1.00	15.74
ATOM	3095	CZ	PHE	248	52.153	86.081	43.227	1.00	17.56
ATOM	3096	C	PHE	248	46.799	82.813	43.977	1.00	25.16

70/145

FIGURE 1 (CONT.)

ATOM	3097	O	PHE	248	45.832	83.469	44.360	1.00	26.87
ATOM	3098	N	THR	249	46.789	81.508	43.969	1.00	23.77
ATOM	3099	H	THR	249	47.492	81.007	43.501	1.00	0.00
ATOM	3100	CA	THR	249	45.713	80.779	44.620	1.00	25.08
ATOM	3101	CB	THR	249	44.925	79.957	43.562	1.00	27.34
ATOM	3102	OG1	THR	249	45.782	79.201	42.709	1.00	25.14
ATOM	3103	HG1	THR	249	45.294	78.405	42.447	1.00	0.00
ATOM	3104	CG2	THR	249	44.143	80.944	42.699	1.00	29.87
ATOM	3105	C	THR	249	46.243	79.879	45.719	1.00	23.78
ATOM	3106	O	THR	249	47.426	79.605	45.737	1.00	24.19
ATOM	3107	N	HIS	250	45.541	79.370	46.720	1.00	25.04
ATOM	3108	H	HIS	250	44.578	79.535	46.722	1.00	0.00
ATOM	3109	CA	HIS	250	46.171	78.551	47.747	1.00	24.41
ATOM	3110	CB	HIS	250	45.232	78.201	48.940	1.00	25.37
ATOM	3111	CG	HIS	250	45.964	77.522	50.121	1.00	27.67
ATOM	3112	CD2	HIS	250	46.894	78.166	50.939	1.00	26.48
ATOM	3113	ND1	HIS	250	45.886	76.240	50.545	1.00	27.34
ATOM	3114	HD1	HIS	250	45.389	75.501	50.129	1.00	0.00
ATOM	3115	CE1	HIS	250	46.715	76.085	51.562	1.00	26.37
ATOM	3116	NE2	HIS	250	47.306	77.242	51.781	1.00	27.51
ATOM	3117	HE2	HIS	250	47.921	77.406	52.523	1.00	0.00
ATOM	3118	C	HIS	250	46.678	77.233	47.202	1.00	24.13
ATOM	3119	O	HIS	250	46.002	76.468	46.540	1.00	22.54
ATOM	3120	N	ASN	251	47.925	76.980	47.530	1.00	25.29
ATOM	3121	H	ASN	251	48.455	77.695	47.929	1.00	0.00
ATOM	3122	CA	ASN	251	48.542	75.735	47.178	1.00	26.17
ATOM	3123	CB	ASN	251	50.041	75.857	47.335	1.00	23.97
ATOM	3124	CG	ASN	251	50.773	74.746	46.628	1.00	22.83
ATOM	3125	OD1	ASN	251	50.526	73.556	46.801	1.00	17.87
ATOM	3126	ND2	ASN	251	51.682	75.066	45.750	1.00	23.87
ATOM	3127	HD21	ASN	251	51.894	76.003	45.590	1.00	0.00
ATOM	3128	HD22	ASN	251	52.080	74.297	45.309	1.00	0.00
ATOM	3129	C	ASN	251	48.016	74.582	48.018	1.00	25.42
ATOM	3130	O	ASN	251	48.349	74.307	49.169	1.00	27.72
ATOM	3131	N	THR	252	47.067	73.934	47.396	1.00	27.21
ATOM	3132	H	THR	252	46.701	74.333	46.575	1.00	0.00
ATOM	3133	CA	THR	252	46.510	72.734	47.974	1.00	27.44
ATOM	3134	CB	THR	252	45.182	72.406	47.249	1.00	28.93
ATOM	3135	OG1	THR	252	44.575	71.305	47.915	1.00	32.62
ATOM	3136	HG1	THR	252	45.237	70.635	48.156	1.00	0.00
ATOM	3137	CG2	THR	252	45.407	72.054	45.772	1.00	32.23
ATOM	3138	C	THR	252	47.517	71.591	47.863	1.00	26.38
ATOM	3139	O	THR	252	47.338	70.661	48.623	1.00	28.38
ATOM	3140	N	VAL	253	48.564	71.538	47.022	1.00	23.72
ATOM	3141	H	VAL	253	48.763	72.310	46.458	1.00	0.00

FIGURE 1 (CONT.)

ATOM	3142	CA	VAL	253	49.501	70.402	47.022	1.00	23.99
ATOM	3143	CB	VAL	253	50.427	70.441	45.755	1.00	23.79
ATOM	3144	CG1	VAL	253	51.588	69.463	45.892	1.00	19.76
ATOM	3145	CG2	VAL	253	49.652	69.997	44.530	1.00	20.79
ATOM	3146	C	VAL	253	50.395	70.379	48.279	1.00	26.73
ATOM	3147	O	VAL	253	50.445	69.410	49.036	1.00	27.90
ATOM	3148	N	ARG	254	51.152	71.469	48.450	1.00	26.41
ATOM	3149	H	ARG	254	51.151	72.104	47.718	1.00	0.00
ATOM	3150	CA	ARG	254	52.013	71.761	49.578	1.00	25.68
ATOM	3151	CB	ARG	254	52.667	73.088	49.354	1.00	26.71
ATOM	3152	CG	ARG	254	53.497	73.266	48.119	1.00	27.49
ATOM	3153	CD	ARG	254	54.678	72.349	48.147	1.00	25.03
ATOM	3154	NE	ARG	254	55.338	72.428	46.874	1.00	21.74
ATOM	3155	HE	ARG	254	55.150	73.178	46.271	1.00	0.00
ATOM	3156	CZ	ARG	254	56.209	71.503	46.510	1.00	20.78
ATOM	3157	NH1	ARG	254	56.755	71.620	45.295	1.00	18.66
ATOM	3158	HH11	ARG	254	57.416	70.938	44.983	1.00	0.00
ATOM	3159	HH12	ARG	254	56.506	72.385	44.700	1.00	0.00
ATOM	3160	NH2	ARG	254	56.581	70.546	47.369	1.00	17.46
ATOM	3161	HH21	ARG	254	56.203	70.517	48.294	1.00	0.00
ATOM	3162	HH22	ARG	254	57.231	69.846	47.080	1.00	0.00
ATOM	3163	C	ARG	254	51.402	71.824	50.996	1.00	27.61
ATOM	3164	O	ARG	254	52.120	71.852	52.016	1.00	26.41
ATOM	3165	N	GLY	255	50.066	72.003	51.077	1.00	28.13
ATOM	3166	H	GLY	255	49.553	71.892	50.253	1.00	0.00
ATOM	3167	CA	GLY	255	49.386	72.232	52.358	1.00	29.13
ATOM	3168	C	GLY	255	49.709	73.615	52.965	1.00	30.08
ATOM	3169	O	GLY	255	49.234	74.021	54.011	1.00	31.93
ATOM	3170	N	CYS	256	50.550	74.399	52.319	1.00	31.22
ATOM	3171	H	CYS	256	51.120	73.968	51.656	1.00	0.00
ATOM	3172	CA	CYS	256	50.912	75.770	52.656	1.00	28.71
ATOM	3173	CB	CYS	256	52.190	75.857	53.461	1.00	31.75
ATOM	3174	SG	CYS	256	53.555	74.911	52.727	1.00	26.89
ATOM	3175	C	CYS	256	51.196	76.485	51.345	1.00	27.09
ATOM	3176	O	CYS	256	51.315	75.891	50.279	1.00	24.12
ATOM	3177	N	SER	257	51.298	77.797	51.421	1.00	26.20
ATOM	3178	H	SER	257	51.220	78.204	52.307	1.00	0.00
ATOM	3179	CA	SER	257	51.603	78.655	50.279	1.00	24.26
ATOM	3180	CB	SER	257	52.973	78.281	49.693	1.00	25.54
ATOM	3181	OG	SER	257	53.496	79.326	48.892	1.00	20.80
ATOM	3182	HG	SER	257	54.404	79.092	48.658	1.00	0.00
ATOM	3183	C	SER	257	50.594	78.716	49.140	1.00	23.11
ATOM	3184	O	SER	257	49.402	78.437	49.364	1.00	20.03
ATOM	3185	N	TYR	258	51.087	79.230	47.994	1.00	21.07
ATOM	3186	H	TYR	258	51.968	79.635	48.013	1.00	0.00

72/145

FIGURE 1 (CONT.)

ATOM	3187	CA	TYR	258	50.413	79.425	46.742	1.00	20.45
ATOM	3188	CB	TYR	258	50.534	80.898	46.378	1.00	23.00
ATOM	3189	CG	TYR	258	49.841	81.721	47.445	1.00	26.87
ATOM	3190	CD1	TYR	258	50.546	82.189	48.554	1.00	26.62
ATOM	3191	CE1	TYR	258	49.851	82.834	49.572	1.00	26.92
ATOM	3192	CD2	TYR	258	48.459	81.916	47.361	1.00	28.03
ATOM	3193	CE2	TYR	258	47.765	82.556	48.360	1.00	23.37
ATOM	3194	CZ	TYR	258	48.475	83.004	49.446	1.00	26.49
ATOM	3195	OH	TYR	258	47.793	83.694	50.413	1.00	32.47
ATOM	3196	HH	TYR	258	46.893	83.869	50.122	1.00	0.00
ATOM	3197	C	TYR	258	50.856	78.580	45.554	1.00	20.26
ATOM	3198	O	TYR	258	51.851	77.868	45.570	1.00	20.06
ATOM	3199	N	PHE	259	49.929	78.586	44.610	1.00	20.62
ATOM	3200	H	PHE	259	49.055	78.955	44.868	1.00	0.00
ATOM	3201	CA	PHE	259	50.040	78.147	43.232	1.00	21.61
ATOM	3202	CB	PHE	259	48.835	77.361	42.749	1.00	18.22
ATOM	3203	CG	PHE	259	48.772	75.886	43.087	1.00	15.28
ATOM	3204	CD1	PHE	259	49.818	75.038	42.724	1.00	15.43
ATOM	3205	CD2	PHE	259	47.660	75.392	43.746	1.00	11.29
ATOM	3206	CE1	PHE	259	49.735	73.680	43.029	1.00	16.32
ATOM	3207	CE2	PHE	259	47.587	74.045	44.040	1.00	11.44
ATOM	3208	CZ	PHE	259	48.614	73.184	43.687	1.00	15.70
ATOM	3209	C	PHE	259	49.987	79.470	42.481	1.00	24.53
ATOM	3210	O	PHE	259	49.055	80.238	42.749	1.00	29.71
ATOM	3211	N	TYR	260	50.884	79.903	41.607	1.00	27.18
ATOM	3212	H	TYR	260	51.671	79.357	41.443	1.00	0.00
ATOM	3213	CA	TYR	260	50.694	81.183	40.887	1.00	29.95
ATOM	3214	CB	TYR	260	51.893	82.145	41.190	1.00	30.03
ATOM	3215	CG	TYR	260	53.288	81.520	41.056	1.00	31.93
ATOM	3216	CD1	TYR	260	53.842	81.377	39.782	1.00	30.21
ATOM	3217	CE1	TYR	260	55.078	80.774	39.621	1.00	33.46
ATOM	3218	CD2	TYR	260	53.976	81.057	42.184	1.00	30.07
ATOM	3219	CE2	TYR	260	55.215	80.443	42.019	1.00	31.96
ATOM	3220	CZ	TYR	260	55.772	80.304	40.734	1.00	34.07
ATOM	3221	OH	TYR	260	57.025	79.729	40.517	1.00	31.76
ATOM	3222	HH	TYR	260	57.424	79.405	41.343	1.00	0.00
ATOM	3223	C	TYR	260	50.494	81.026	39.359	1.00	32.49
ATOM	3224	O	TYR	260	50.893	80.026	38.713	1.00	33.88
ATOM	3225	N	SER	261	49.863	82.039	38.747	1.00	32.05
ATOM	3226	H	SER	261	49.666	82.823	39.296	1.00	0.00
ATOM	3227	CA	SER	261	49.474	81.992	37.335	1.00	27.70
ATOM	3228	CB	SER	261	48.102	82.610	37.142	1.00	27.77
ATOM	3229	OG	SER	261	47.971	84.054	37.229	1.00	24.36
ATOM	3230	HG	SER	261	47.335	84.218	36.521	1.00	0.00
ATOM	3231	C	SER	261	50.394	82.686	36.361	1.00	27.85

73/145

FIGURE 1 (CONT.)

ATOM	3232	O	SER	261	51.272	83.440	36.774	1.00	27.95
ATOM	3233	N	TYR	262	50.202	82.489	35.047	1.00	28.67
ATOM	3234	H	TYR	262	49.577	81.783	34.773	1.00	0.00
ATOM	3235	CA	TYR	262	50.957	83.199	34.030	1.00	27.65
ATOM	3236	CB	TYR	262	50.671	82.537	32.702	1.00	27.21
ATOM	3237	CG	TYR	262	51.203	83.219	31.452	1.00	29.56
ATOM	3238	CD1	TYR	262	52.566	83.342	31.193	1.00	30.15
ATOM	3239	CE1	TYR	262	52.997	83.992	30.042	1.00	31.58
ATOM	3240	CD2	TYR	262	50.277	83.738	30.560	1.00	30.20
ATOM	3241	CE2	TYR	262	50.707	84.391	29.414	1.00	31.66
ATOM	3242	CZ	TYR	262	52.058	84.523	29.155	1.00	33.65
ATOM	3243	OH	TYR	262	52.430	85.238	28.017	1.00	37.67
ATOM	3244	HH	TYR	262	53.358	85.056	27.809	1.00	0.00
ATOM	3245	C	TYR	262	50.598	84.676	34.030	1.00	29.66
ATOM	3246	O	TYR	262	51.540	85.473	34.002	1.00	33.39
ATOM	3247	N	PRO	263	49.338	85.154	34.168	1.00	29.59
ATOM	3248	CD	PRO	263	48.104	84.466	33.770	1.00	28.28
ATOM	3249	CA	PRO	263	49.028	86.485	34.699	1.00	28.70
ATOM	3250	CB	PRO	263	47.575	86.419	35.038	1.00	28.27
ATOM	3251	CG	PRO	263	47.027	85.508	33.953	1.00	29.80
ATOM	3252	C	PRO	263	49.854	86.935	35.894	1.00	30.47
ATOM	3253	O	PRO	263	50.193	88.109	35.975	1.00	33.15
ATOM	3254	N	ALA	264	50.170	86.113	36.907	1.00	31.52
ATOM	3255	H	ALA	264	49.891	85.173	36.880	1.00	0.00
ATOM	3256	CA	ALA	264	51.037	86.569	37.995	1.00	29.68
ATOM	3257	CB	ALA	264	51.114	85.594	39.159	1.00	29.65
ATOM	3258	C	ALA	264	52.469	86.766	37.524	1.00	29.91
ATOM	3259	O	ALA	264	52.919	87.927	37.574	1.00	28.83
ATOM	3260	N	VAL	265	53.186	85.749	36.986	1.00	27.83
ATOM	3261	H	VAL	265	52.774	84.869	36.852	1.00	0.00
ATOM	3262	CA	VAL	265	54.586	86.033	36.666	1.00	26.54
ATOM	3263	CB	VAL	265	55.458	84.789	36.229	1.00	24.65
ATOM	3264	CG1	VAL	265	55.113	83.668	37.156	1.00	26.80
ATOM	3265	CG2	VAL	265	55.210	84.285	34.861	1.00	28.18
ATOM	3266	C	VAL	265	54.672	87.084	35.575	1.00	26.85
ATOM	3267	O	VAL	265	55.445	88.027	35.769	1.00	27.45
ATOM	3268	N	CYS	266	53.837	87.128	34.523	1.00	26.17
ATOM	3269	H	CYS	266	53.158	86.432	34.426	1.00	0.00
ATOM	3270	CA	CYS	266	53.991	88.205	33.536	1.00	24.92
ATOM	3271	CB	CYS	266	53.042	87.929	32.323	1.00	24.54
ATOM	3272	SG	CYS	266	53.871	87.357	30.790	1.00	27.09
ATOM	3273	C	CYS	266	53.753	89.587	34.175	1.00	23.76
ATOM	3274	O	CYS	266	54.407	90.553	33.806	1.00	26.29
ATOM	3275	N	GLU	267	52.975	89.740	35.242	1.00	23.60
ATOM	3276	H	GLU	267	52.442	88.968	35.525	1.00	0.00

74/145

FIGURE 1 (CONT.)

ATOM	3277	CA	GLU	267	52.849	91.000	36.002	1.00	25.10
ATOM	3278	CB	GLU	267	51.648	90.892	36.943	1.00	27.58
ATOM	3279	CG	GLU	267	51.425	91.990	37.980	1.00	32.71
ATOM	3280	CD	GLU	267	51.514	93.403	37.422	1.00	36.74
ATOM	3281	OE1	GLU	267	52.377	94.187	37.845	1.00	38.60
ATOM	3282	OE2	GLU	267	50.720	93.713	36.544	1.00	40.70
ATOM	3283	C	GLU	267	54.090	91.374	36.830	1.00	26.56
ATOM	3284	O	GLU	267	54.514	92.538	36.909	1.00	27.89
ATOM	3285	N	PHE	268	54.703	90.380	37.478	1.00	26.49
ATOM	3286	H	PHE	268	54.265	89.502	37.429	1.00	0.00
ATOM	3287	CA	PHE	268	55.959	90.522	38.224	1.00	24.12
ATOM	3288	CB	PHE	268	56.437	89.184	38.850	1.00	24.61
ATOM	3289	CG	PHE	268	57.564	89.378	39.851	1.00	21.69
ATOM	3290	CD1	PHE	268	57.249	89.900	41.111	1.00	19.96
ATOM	3291	CD2	PHE	268	58.890	89.153	39.480	1.00	20.60
ATOM	3292	CE1	PHE	268	58.263	90.228	41.998	1.00	17.34
ATOM	3293	CE2	PHE	268	59.893	89.489	40.390	1.00	23.36
ATOM	3294	CZ	PHE	268	59.583	90.032	41.639	1.00	19.55
ATOM	3295	C	PHE	268	57.053	90.973	37.287	1.00	24.28
ATOM	3296	O	PHE	268	57.746	91.957	37.544	1.00	25.43
ATOM	3297	N	LEU	269	57.161	90.230	36.180	1.00	25.16
ATOM	3298	H	LEU	269	56.546	89.474	36.111	1.00	0.00
ATOM	3299	CA	LEU	269	58.124	90.446	35.090	1.00	26.95
ATOM	3300	CB	LEU	269	57.924	89.332	34.041	1.00	23.08
ATOM	3301	CG	LEU	269	58.282	87.949	34.559	1.00	17.37
ATOM	3302	CD1	LEU	269	58.168	86.883	33.484	1.00	18.64
ATOM	3303	CD2	LEU	269	59.726	87.997	35.034	1.00	19.21
ATOM	3304	C	LEU	269	58.035	91.833	34.431	1.00	30.69
ATOM	3305	O	LEU	269	59.029	92.576	34.400	1.00	33.53
ATOM	3306	N	GLN	270	56.846	92.272	33.985	1.00	30.63
ATOM	3307	H	GLN	270	56.099	91.634	33.952	1.00	0.00
ATOM	3308	CA	GLN	270	56.684	93.640	33.492	1.00	30.29
ATOM	3309	CB	GLN	270	55.298	93.833	32.904	1.00	32.88
ATOM	3310	CG	GLN	270	55.184	92.796	31.785	1.00	37.43
ATOM	3311	CD	GLN	270	53.952	92.783	30.912	1.00	36.41
ATOM	3312	OE1	GLN	270	52.829	92.922	31.360	1.00	37.69
ATOM	3313	NE2	GLN	270	54.106	92.587	29.622	1.00	37.81
ATOM	3314	HE21	GLN	270	55.005	92.422	29.278	1.00	0.00
ATOM	3315	HE22	GLN	270	53.273	92.581	29.123	1.00	0.00
ATOM	3316	C	GLN	270	56.893	94.642	34.618	1.00	29.71
ATOM	3317	O	GLN	270	57.685	95.568	34.465	1.00	28.91
ATOM	3318	N	HIS	271	56.330	94.445	35.817	1.00	28.81
ATOM	3319	H	HIS	271	55.769	93.649	35.940	1.00	0.00
ATOM	3320	CA	HIS	271	56.524	95.420	36.886	1.00	28.70
ATOM	3321	CB	HIS	271	55.679	95.063	38.070	1.00	30.20

75/145

FIGURE 1 (CONT.)

ATOM	3322	CG	HIS	271	55.546	96.214	39.057	1.00	32.78
ATOM	3323	CD2	HIS	271	56.433	96.536	40.062	1.00	33.83
ATOM	3324	ND1	HIS	271	54.565	97.102	39.098	1.00	34.76
ATOM	3325	HD1	HIS	271	53.777	97.138	38.516	1.00	0.00
ATOM	3326	CE1	HIS	271	54.825	97.940	40.073	1.00	35.78
ATOM	3327	NE2	HIS	271	55.948	97.595	40.645	1.00	33.48
ATOM	3328	HE2	HIS	271	56.380	98.072	41.382	1.00	0.00
ATOM	3329	C	HIS	271	57.947	95.638	37.409	1.00	28.94
ATOM	3330	O	HIS	271	58.319	96.699	37.925	1.00	28.66
ATOM	3331	N	ASN	272	58.727	94.575	37.392	1.00	30.67
ATOM	3332	H	ASN	272	58.367	93.725	37.070	1.00	0.00
ATOM	3333	CA	ASN	272	60.098	94.685	37.844	1.00	29.80
ATOM	3334	CB	ASN	272	60.296	93.476	38.707	1.00	29.16
ATOM	3335	CG	ASN	272	59.481	93.663	39.990	1.00	29.43
ATOM	3336	OD1	ASN	272	59.870	94.372	40.913	1.00	27.49
ATOM	3337	ND2	ASN	272	58.308	93.094	40.164	1.00	26.58
ATOM	3338	HD21	ASN	272	57.954	92.534	39.450	1.00	0.00
ATOM	3339	HD22	ASN	272	57.879	93.288	41.023	1.00	0.00
ATOM	3340	C	ASN	272	61.148	94.841	36.729	1.00	29.95
ATOM	3341	O	ASN	272	62.320	95.072	37.012	1.00	30.29
ATOM	3342	N	ASN	273	60.696	94.821	35.456	1.00	28.09
ATOM	3343	H	ASN	273	59.726	94.794	35.332	1.00	0.00
ATOM	3344	CA	ASN	273	61.509	94.928	34.248	1.00	27.15
ATOM	3345	CB	ASN	273	62.210	96.314	34.191	1.00	29.71
ATOM	3346	CG	ASN	273	63.067	96.607	32.956	1.00	31.42
ATOM	3347	OD1	ASN	273	62.682	96.337	31.822	1.00	31.34
ATOM	3348	ND2	ASN	273	64.269	97.163	33.050	1.00	29.17
ATOM	3349	HD21	ASN	273	64.643	97.366	33.925	1.00	0.00
ATOM	3350	HD22	ASN	273	64.694	97.288	32.182	1.00	0.00
ATOM	3351	C	ASN	273	62.511	93.795	34.232	1.00	26.12
ATOM	3352	O	ASN	273	63.736	93.894	34.158	1.00	25.90
ATOM	3353	N	LEU	274	61.871	92.654	34.356	1.00	25.36
ATOM	3354	H	LEU	274	60.899	92.685	34.410	1.00	0.00
ATOM	3355	CA	LEU	274	62.575	91.379	34.356	1.00	25.44
ATOM	3356	CB	LEU	274	62.297	90.650	35.676	1.00	23.63
ATOM	3357	CG	LEU	274	62.733	91.179	37.023	1.00	21.66
ATOM	3358	CD1	LEU	274	62.117	90.271	38.045	1.00	17.73
ATOM	3359	CD2	LEU	274	64.256	91.158	37.214	1.00	18.97
ATOM	3360	C	LEU	274	62.256	90.420	33.199	1.00	22.88
ATOM	3361	O	LEU	274	61.144	90.327	32.685	1.00	24.51
ATOM	3362	N	LEU	275	63.204	89.614	32.767	1.00	22.83
ATOM	3363	H	LEU	275	64.078	89.671	33.206	1.00	0.00
ATOM	3364	CA	LEU	275	62.962	88.641	31.713	1.00	21.29
ATOM	3365	CB	LEU	275	64.291	88.316	31.126	1.00	20.41
ATOM	3366	CG	LEU	275	64.251	87.576	29.845	1.00	20.28

76/145

**FIGURE 1 (CONT.)**

ATOM	3367	CD1	LEU	275	63.515	88.416	28.843	1.00	23.16
ATOM	3368	CD2	LEU	275	65.642	87.263	29.398	1.00	22.33
ATOM	3369	C	LEU	275	62.228	87.332	32.063	1.00	22.03
ATOM	3370	O	LEU	275	61.350	86.847	31.340	1.00	20.34
ATOM	3371	N	SER	276	62.597	86.701	33.182	1.00	21.44
ATOM	3372	H	SER	276	63.194	87.156	33.810	1.00	0.00
ATOM	3373	CA	SER	276	62.039	85.401	33.526	1.00	19.63
ATOM	3374	CB	SER	276	62.721	84.331	32.704	1.00	15.72
ATOM	3375	OG	SER	276	62.116	83.052	32.739	1.00	16.88
ATOM	3376	HG	SER	276	61.522	82.973	31.975	1.00	0.00
ATOM	3377	C	SER	276	62.208	85.072	34.999	1.00	21.13
ATOM	3378	O	SER	276	62.977	85.756	35.676	1.00	22.01
ATOM	3379	N	ILE	277	61.478	84.074	35.523	1.00	20.71
ATOM	3380	H	ILE	277	60.779	83.699	34.942	1.00	0.00
ATOM	3381	CA	ILE	277	61.647	83.534	36.879	1.00	18.06
ATOM	3382	CB	ILE	277	60.293	83.382	37.699	1.00	17.47
ATOM	3383	CG2	ILE	277	60.617	82.768	39.051	1.00	16.09
ATOM	3384	CG1	ILE	277	59.551	84.707	37.888	1.00	14.46
ATOM	3385	CD1	ILE	277	60.368	85.947	38.246	1.00	16.30
ATOM	3386	C	ILE	277	62.257	82.135	36.774	1.00	17.20
ATOM	3387	O	ILE	277	61.589	81.167	36.375	1.00	17.80
ATOM	3388	N	LEU	278	63.549	82.030	37.117	1.00	17.25
ATOM	3389	H	LEU	278	63.997	82.831	37.455	1.00	0.00
ATOM	3390	CA	LEU	278	64.232	80.733	37.145	1.00	16.64
ATOM	3391	CB	LEU	278	65.731	80.753	36.872	1.00	17.64
ATOM	3392	CG	LEU	278	66.328	81.501	35.707	1.00	19.09
ATOM	3393	CD1	LEU	278	67.688	80.900	35.386	1.00	20.10
ATOM	3394	CD2	LEU	278	65.428	81.391	34.509	1.00	19.63
ATOM	3395	C	LEU	278	64.114	80.161	38.543	1.00	16.12
ATOM	3396	O	LEU	278	64.436	80.761	39.560	1.00	17.50
ATOM	3397	N	ARG	279	63.580	78.967	38.603	1.00	15.53
ATOM	3398	H	ARG	279	63.350	78.492	37.777	1.00	0.00
ATOM	3399	CA	ARG	279	63.251	78.368	39.872	1.00	13.35
ATOM	3400	CB	ARG	279	61.813	78.741	40.177	1.00	10.64
ATOM	3401	CG	ARG	279	60.836	78.057	39.257	1.00	8.14
ATOM	3402	CD	ARG	279	59.826	77.608	40.216	1.00	13.27
ATOM	3403	NE	ARG	279	59.390	76.270	39.952	1.00	14.83
ATOM	3404	HE	ARG	279	59.696	75.807	39.146	1.00	0.00
ATOM	3405	CZ	ARG	279	58.577	75.644	40.806	1.00	14.31
ATOM	3406	NH1	ARG	279	58.227	74.415	40.504	1.00	16.84
ATOM	3407	HH11	ARG	279	57.642	73.910	41.133	1.00	0.00
ATOM	3408	HH12	ARG	279	58.571	73.986	39.668	1.00	0.00
ATOM	3409	NH2	ARG	279	58.111	76.169	41.939	1.00	8.13
ATOM	3410	HH21	ARG	279	58.375	77.089	42.211	1.00	0.00
ATOM	3411	HH22	ARG	279	57.508	75.626	42.525	1.00	0.00

77/145

FIGURE 1 (CONT.)

ATOM	3412	C	ARG	279	63.439	76.861	39.777	1.00	14.44
ATOM	3413	O	ARG	279	63.702	76.330	38.686	1.00	14.64
ATOM	3414	N	ALA	280	63.267	76.144	40.883	1.00	14.07
ATOM	3415	H	ALA	280	62.978	76.627	41.683	1.00	0.00
ATOM	3416	CA	ALA	280	63.462	74.698	40.886	1.00	14.65
ATOM	3417	CB	ALA	280	64.780	74.472	41.623	1.00	7.95
ATOM	3418	C	ALA	280	62.258	74.009	41.557	1.00	16.36
ATOM	3419	O	ALA	280	61.137	74.159	41.087	1.00	18.11
ATOM	3420	N	HIS	281	62.399	73.167	42.608	1.00	18.12
ATOM	3421	H	HIS	281	63.297	72.817	42.678	1.00	0.00
ATOM	3422	CA	HIS	281	61.353	72.685	43.540	1.00	15.72
ATOM	3423	CB	HIS	281	60.577	73.888	44.014	1.00	15.93
ATOM	3424	CG	HIS	281	59.586	73.858	45.164	1.00	19.33
ATOM	3425	CD2	HIS	281	58.487	74.703	45.165	1.00	18.95
ATOM	3426	ND1	HIS	281	59.580	73.199	46.312	1.00	21.77
ATOM	3427	HD1	HIS	281	59.943	72.307	46.441	1.00	0.00
ATOM	3428	CE1	HIS	281	58.543	73.629	46.994	1.00	21.06
ATOM	3429	NE2	HIS	281	57.899	74.524	46.294	1.00	20.13
ATOM	3430	HE2	HIS	281	57.054	74.952	46.552	1.00	0.00
ATOM	3431	C	HIS	281	60.392	71.625	43.081	1.00	15.77
ATOM	3432	O	HIS	281	59.853	70.886	43.890	1.00	15.52
ATOM	3433	N	GLU	282	60.194	71.601	41.782	1.00	17.89
ATOM	3434	H	GLU	282	60.568	72.323	41.241	1.00	0.00
ATOM	3435	CA	GLU	282	59.370	70.645	41.091	1.00	18.03
ATOM	3436	CB	GLU	282	58.439	71.412	40.240	1.00	18.88
ATOM	3437	CG	GLU	282	57.044	70.972	40.520	1.00	22.26
ATOM	3438	CD	GLU	282	56.294	72.174	40.965	1.00	20.86
ATOM	3439	OE1	GLU	282	56.314	72.405	42.162	1.00	27.50
ATOM	3440	OE2	GLU	282	55.777	72.890	40.129	1.00	17.91
ATOM	3441	C	GLU	282	60.096	69.607	40.227	1.00	18.08
ATOM	3442	O	GLU	282	60.710	69.910	39.193	1.00	18.00
ATOM	3443	N	ALA	283	59.979	68.353	40.667	1.00	16.31
ATOM	3444	H	ALA	283	59.466	68.218	41.488	1.00	0.00
ATOM	3445	CA	ALA	283	60.556	67.221	39.972	1.00	15.14
ATOM	3446	CB	ALA	283	60.035	65.932	40.549	1.00	12.58
ATOM	3447	C	ALA	283	60.222	67.246	38.507	1.00	14.53
ATOM	3448	O	ALA	283	59.063	67.360	38.228	1.00	16.04
ATOM	3449	N	GLN	284	61.144	67.301	37.551	1.00	18.04
ATOM	3450	H	GLN	284	62.076	67.415	37.819	1.00	0.00
ATOM	3451	CA	GLN	284	60.813	67.219	36.136	1.00	16.76
ATOM	3452	CB	GLN	284	61.295	68.412	35.361	1.00	17.57
ATOM	3453	CG	GLN	284	60.760	69.776	35.727	1.00	19.06
ATOM	3454	CD	GLN	284	59.257	69.875	35.711	1.00	18.59
ATOM	3455	OE1	GLN	284	58.596	69.756	34.711	1.00	20.73
ATOM	3456	NE2	GLN	284	58.574	70.056	36.798	1.00	22.84

78/145

FIGURE 1 (CONT.)

ATOM	3457	HE21	GLN	284	57.614	70.115	36.647	1.00	0.00
ATOM	3458	HE22	GLN	284	59.049	70.124	37.647	1.00	0.00
ATOM	3459	C	GLN	284	61.446	66.005	35.483	1.00	18.81
ATOM	3460	O	GLN	284	62.559	65.555	35.757	1.00	20.97
ATOM	3461	N	ASP	285	60.728	65.459	34.537	1.00	20.00
ATOM	3462	H	ASP	285	59.842	65.842	34.360	1.00	0.00
ATOM	3463	CA	ASP	285	61.171	64.270	33.830	1.00	22.02
ATOM	3464	CB	ASP	285	60.013	63.788	32.984	1.00	27.23
ATOM	3465	CG	ASP	285	60.053	62.290	32.956	1.00	32.95
ATOM	3466	OD1	ASP	285	59.334	61.719	33.781	1.00	39.86
ATOM	3467	OD2	ASP	285	60.823	61.730	32.159	1.00	36.01
ATOM	3468	C	ASP	285	62.420	64.399	32.970	1.00	19.72
ATOM	3469	O	ASP	285	63.255	63.510	32.967	1.00	20.36
ATOM	3470	N	GLY	286	62.497	65.490	32.197	1.00	20.09
ATOM	3471	H	GLY	286	61.683	66.027	32.121	1.00	0.00
ATOM	3472	CA	GLY	286	63.678	65.868	31.432	1.00	18.31
ATOM	3473	C	GLY	286	64.637	66.694	32.306	1.00	21.16
ATOM	3474	O	GLY	286	65.546	67.382	31.833	1.00	24.21
ATOM	3475	N	GLY	287	64.470	66.710	33.629	1.00	20.95
ATOM	3476	H	GLY	287	63.925	66.021	34.063	1.00	0.00
ATOM	3477	CA	GLY	287	65.247	67.581	34.504	1.00	17.89
ATOM	3478	C	GLY	287	64.964	69.062	34.407	1.00	14.88
ATOM	3479	O	GLY	287	65.444	69.775	35.257	1.00	15.62
ATOM	3480	N	TYR	288	64.225	69.588	33.438	1.00	14.85
ATOM	3481	H	TYR	288	63.920	68.986	32.735	1.00	0.00
ATOM	3482	CA	TYR	288	63.914	71.012	33.267	1.00	15.02
ATOM	3483	CB	TYR	288	64.950	71.729	32.364	1.00	14.57
ATOM	3484	CG	TYR	288	64.862	71.390	30.866	1.00	17.21
ATOM	3485	CD1	TYR	288	65.262	70.123	30.388	1.00	18.76
ATOM	3486	CE1	TYR	288	65.148	69.807	29.026	1.00	16.60
ATOM	3487	CD2	TYR	288	64.355	72.340	29.955	1.00	17.61
ATOM	3488	CE2	TYR	288	64.251	72.038	28.589	1.00	15.87
ATOM	3489	CZ	TYR	288	64.642	70.774	28.148	1.00	18.39
ATOM	3490	OH	TYR	288	64.505	70.464	26.807	1.00	26.73
ATOM	3491	HH	TYR	288	64.823	69.565	26.665	1.00	0.00
ATOM	3492	C	TYR	288	62.539	71.208	32.617	1.00	15.28
ATOM	3493	O	TYR	288	61.982	70.295	32.033	1.00	16.05
ATOM	3494	N	ARG	289	61.963	72.396	32.639	1.00	17.42
ATOM	3495	H	ARG	289	62.397	73.070	33.209	1.00	0.00
ATOM	3496	CA	ARG	289	60.707	72.739	31.974	1.00	17.90
ATOM	3497	CB	ARG	289	59.574	72.352	32.876	1.00	19.13
ATOM	3498	CG	ARG	289	58.238	72.932	32.508	1.00	23.08
ATOM	3499	CD	ARG	289	57.350	71.821	32.190	1.00	24.89
ATOM	3500	NE	ARG	289	56.217	71.817	33.051	1.00	27.20
ATOM	3501	HE	ARG	289	56.272	71.424	33.948	1.00	0.00

FIGURE 1 (CONT.)

ATOM	3502	CZ	ARG	289	55.069	72.312	32.614	1.00	32.35
ATOM	3503	NH1	ARG	289	53.980	72.136	33.385	1.00	35.22
ATOM	3504	HH11	ARG	289	54.060	71.644	34.251	1.00	0.00
ATOM	3505	HH12	ARG	289	53.094	72.498	33.094	1.00	0.00
ATOM	3506	NH2	ARG	289	54.991	73.016	31.465	1.00	33.43
ATOM	3507	HH21	ARG	289	55.802	73.169	30.903	1.00	0.00
ATOM	3508	HH22	ARG	289	54.105	73.368	31.167	1.00	0.00
ATOM	3509	C	ARG	289	60.619	74.234	31.648	1.00	19.75
ATOM	3510	O	ARG	289	60.809	75.123	32.485	1.00	18.68
ATOM	3511	N	MET	290	60.339	74.560	30.397	1.00	22.37
ATOM	3512	H	MET	290	60.124	73.841	29.772	1.00	0.00
ATOM	3513	CA	MET	290	60.195	75.963	29.974	1.00	23.15
ATOM	3514	CB	MET	290	60.774	76.156	28.564	1.00	22.09
ATOM	3515	CG	MET	290	62.258	75.973	28.366	1.00	19.95
ATOM	3516	SD	MET	290	63.167	77.381	29.026	1.00	28.66
ATOM	3517	CE	MET	290	64.822	76.799	29.289	1.00	24.57
ATOM	3518	C	MET	290	58.697	76.327	29.973	1.00	24.22
ATOM	3519	O	MET	290	57.865	75.551	29.490	1.00	26.56
ATOM	3520	N	TYR	291	58.221	77.424	30.529	1.00	23.54
ATOM	3521	H	TYR	291	58.838	78.049	30.965	1.00	0.00
ATOM	3522	CA	TYR	291	56.780	77.650	30.511	1.00	22.89
ATOM	3523	CB	TYR	291	56.285	78.153	31.942	1.00	22.49
ATOM	3524	CG	TYR	291	56.457	77.112	33.047	1.00	18.53
ATOM	3525	CD1	TYR	291	55.367	76.443	33.581	1.00	18.70
ATOM	3526	CE1	TYR	291	55.594	75.385	34.467	1.00	20.79
ATOM	3527	CD2	TYR	291	57.739	76.744	33.416	1.00	18.28
ATOM	3528	CE2	TYR	291	57.969	75.697	34.298	1.00	18.50
ATOM	3529	CZ	TYR	291	56.897	75.002	34.827	1.00	18.93
ATOM	3530	OH	TYR	291	57.137	73.919	35.668	1.00	15.29
ATOM	3531	HH	TYR	291	58.025	74.010	36.042	1.00	0.00
ATOM	3532	C	TYR	291	56.408	78.641	29.425	1.00	24.16
ATOM	3533	O	TYR	291	57.254	79.165	28.701	1.00	22.65
ATOM	3534	N	ARG	292	55.115	78.944	29.337	1.00	26.89
ATOM	3535	H	ARG	292	54.496	78.465	29.923	1.00	0.00
ATOM	3536	CA	ARG	292	54.599	79.941	28.404	1.00	29.05
ATOM	3537	CB	ARG	292	53.177	80.332	28.857	1.00	29.32
ATOM	3538	CG	ARG	292	52.563	81.057	27.676	1.00	27.54
ATOM	3539	CD	ARG	292	51.078	80.980	27.658	1.00	25.70
ATOM	3540	NE	ARG	292	50.636	81.894	26.629	1.00	25.94
ATOM	3541	HE	ARG	292	51.181	82.032	25.826	1.00	0.00
ATOM	3542	CZ	ARG	292	49.489	82.546	26.744	1.00	28.62
ATOM	3543	NH1	ARG	292	49.189	83.398	25.775	1.00	32.49
ATOM	3544	HH11	ARG	292	49.804	83.507	24.994	1.00	0.00
ATOM	3545	HH12	ARG	292	48.321	83.894	25.805	1.00	0.00
ATOM	3546	NH2	ARG	292	48.640	82.375	27.780	1.00	30.70

FIGURE 1 (CONT.)

ATOM	3547	HH21	ARG	292	48.856	81.738	28.519	1.00	0.00
ATOM	3548	HH22	ARG	292	47.784	82.892	27.806	1.00	0.00
ATOM	3549	C	ARG	292	55.444	81.201	28.195	1.00	29.50
ATOM	3550	O	ARG	292	55.742	81.927	29.148	1.00	32.32
ATOM	3551	N	LYS	293	55.906	81.385	26.943	1.00	30.05
ATOM	3552	H	LYS	293	55.666	80.696	26.292	1.00	0.00
ATOM	3553	CA	LYS	293	56.784	82.501	26.530	1.00	28.64
ATOM	3554	CB	LYS	293	57.177	82.307	25.055	1.00	29.25
ATOM	3555	CG	LYS	293	58.234	81.231	24.898	1.00	30.03
ATOM	3556	CD	LYS	293	58.771	81.061	23.486	1.00	33.20
ATOM	3557	CE	LYS	293	59.703	79.813	23.332	1.00	37.50
ATOM	3558	NZ	LYS	293	61.127	79.916	23.684	1.00	36.16
ATOM	3559	HZ1	LYS	293	61.220	80.221	24.675	1.00	0.00
ATOM	3560	HZ2	LYS	293	61.585	80.610	23.060	1.00	0.00
ATOM	3561	HZ3	LYS	293	61.587	78.991	23.568	1.00	0.00
ATOM	3562	C	LYS	293	56.217	83.905	26.730	1.00	27.12
ATOM	3563	O	LYS	293	55.001	84.041	26.813	1.00	28.76
ATOM	3564	N	SER	294	56.967	84.981	26.825	1.00	26.42
ATOM	3565	H	SER	294	57.941	84.885	26.772	1.00	0.00
ATOM	3566	CA	SER	294	56.372	86.281	27.097	1.00	26.77
ATOM	3567	CB	SER	294	57.406	87.292	27.576	1.00	26.90
ATOM	3568	OG	SER	294	57.066	88.648	27.894	1.00	21.66
ATOM	3569	HG	SER	294	56.518	89.078	27.218	1.00	0.00
ATOM	3570	C	SER	294	55.637	86.978	25.983	1.00	30.85
ATOM	3571	O	SER	294	55.229	88.095	26.276	1.00	35.97
ATOM	3572	N	GLN	295	55.334	86.551	24.740	1.00	31.67
ATOM	3573	H	GLN	295	55.555	85.630	24.514	1.00	0.00
ATOM	3574	CA	GLN	295	54.682	87.433	23.709	1.00	30.98
ATOM	3575	CB	GLN	295	53.229	87.875	24.148	1.00	29.89
ATOM	3576	CG	GLN	295	52.063	87.039	23.616	1.00	32.09
ATOM	3577	CD	GLN	295	51.743	87.270	22.137	1.00	34.28
ATOM	3578	OE1	GLN	295	51.781	86.379	21.313	1.00	37.34
ATOM	3579	NE2	GLN	295	51.384	88.405	21.578	1.00	37.52
ATOM	3580	HE21	GLN	295	51.260	89.205	22.117	1.00	0.00
ATOM	3581	HE22	GLN	295	51.236	88.310	20.619	1.00	0.00
ATOM	3582	C	GLN	295	55.484	88.715	23.363	1.00	28.54
ATOM	3583	O	GLN	295	56.154	88.850	22.356	1.00	25.42
ATOM	3584	N	THR	296	55.488	89.676	24.270	1.00	30.60
ATOM	3585	H	THR	296	54.956	89.492	25.072	1.00	0.00
ATOM	3586	CA	THR	296	56.222	90.946	24.251	1.00	32.14
ATOM	3587	CB	THR	296	55.837	91.725	25.470	1.00	34.89
ATOM	3588	OG1	THR	296	56.395	91.005	26.582	1.00	38.56
ATOM	3589	HG1	THR	296	56.506	91.496	27.414	1.00	0.00
ATOM	3590	CG2	THR	296	54.297	91.822	25.643	1.00	36.02
ATOM	3591	C	THR	296	57.728	90.819	24.231	1.00	33.39

81/145

FIGURE 1 (CONT.)

ATOM	3592	O	THR	296	58.465	91.806	24.195	1.00	36.52
ATOM	3593	N	THR	297	58.150	89.592	24.540	1.00	33.35
ATOM	3594	H	THR	297	57.489	89.033	24.995	1.00	0.00
ATOM	3595	CA	THR	297	59.505	89.055	24.368	1.00	32.44
ATOM	3596	CB	THR	297	60.478	89.035	25.627	1.00	32.41
ATOM	3597	OG1	THR	297	60.317	87.806	26.346	1.00	32.84
ATOM	3598	HG1	THR	297	60.118	87.979	27.283	1.00	0.00
ATOM	3599	CG2	THR	297	60.263	90.252	26.511	1.00	33.29
ATOM	3600	C	THR	297	59.216	87.586	24.026	1.00	33.78
ATOM	3601	O	THR	297	58.165	87.035	24.427	1.00	35.63
ATOM	3602	N	GLY	298	60.060	86.841	23.311	1.00	30.43
ATOM	3603	H	GLY	298	60.903	87.215	22.992	1.00	0.00
ATOM	3604	CA	GLY	298	59.644	85.476	22.970	1.00	27.91
ATOM	3605	C	GLY	298	60.326	84.428	23.810	1.00	26.58
ATOM	3606	O	GLY	298	60.603	83.324	23.369	1.00	26.80
ATOM	3607	N	PHE	299	60.578	84.772	25.060	1.00	27.46
ATOM	3608	H	PHE	299	60.256	85.643	25.374	1.00	0.00
ATOM	3609	CA	PHE	299	61.333	83.918	25.984	1.00	25.78
ATOM	3610	CB	PHE	299	62.424	84.860	26.560	1.00	24.19
ATOM	3611	CG	PHE	299	63.481	84.089	27.315	1.00	22.71
ATOM	3612	CD1	PHE	299	64.496	83.452	26.611	1.00	20.47
ATOM	3613	CD2	PHE	299	63.407	83.986	28.699	1.00	22.01
ATOM	3614	CE1	PHE	299	65.454	82.697	27.277	1.00	18.37
ATOM	3615	CE2	PHE	299	64.371	83.229	29.345	1.00	22.41
ATOM	3616	CZ	PHE	299	65.393	82.584	28.644	1.00	20.57
ATOM	3617	C	PHE	299	60.443	83.236	27.070	1.00	24.34
ATOM	3618	O	PHE	299	59.445	83.875	27.449	1.00	23.78
ATOM	3619	N	PRO	300	60.640	82.013	27.632	1.00	21.90
ATOM	3620	CD	PRO	300	61.661	81.046	27.241	1.00	19.41
ATOM	3621	CA	PRO	300	59.741	81.424	28.640	1.00	21.55
ATOM	3622	CB	PRO	300	60.439	80.126	29.008	1.00	18.91
ATOM	3623	CG	PRO	300	61.077	79.728	27.722	1.00	18.30
ATOM	3624	C	PRO	300	59.456	82.346	29.843	1.00	22.51
ATOM	3625	O	PRO	300	60.422	82.909	30.377	1.00	25.12
ATOM	3626	N	SER	301	58.223	82.630	30.299	1.00	21.04
ATOM	3627	H	SER	301	57.451	82.263	29.830	1.00	0.00
ATOM	3628	CA	SER	301	58.040	83.519	31.467	1.00	21.06
ATOM	3629	CB	SER	301	56.604	83.918	31.575	1.00	16.89
ATOM	3630	OG	SER	301	55.854	82.730	31.735	1.00	20.09
ATOM	3631	HG	SER	301	55.375	82.580	30.905	1.00	0.00
ATOM	3632	C	SER	301	58.492	82.926	32.832	1.00	20.40
ATOM	3633	O	SER	301	58.873	83.615	33.783	1.00	20.81
ATOM	3634	N	LEU	302	58.537	81.594	32.876	1.00	19.95
ATOM	3635	H	LEU	302	58.153	81.150	32.098	1.00	0.00
ATOM	3636	CA	LEU	302	59.024	80.756	33.977	1.00	17.90

FIGURE 1 (CONT.)

ATOM	3637	CB	LEU	302	57.838	80.182	34.757	1.00	14.34
ATOM	3638	CG	LEU	302	58.029	79.405	36.043	1.00	9.24
ATOM	3639	CD1	LEU	302	58.428	80.277	37.178	1.00	7.80
ATOM	3640	CD2	LEU	302	56.726	78.774	36.376	1.00	9.67
ATOM	3641	C	LEU	302	59.902	79.590	33.474	1.00	17.95
ATOM	3642	O	LEU	302	59.687	79.062	32.377	1.00	16.22
ATOM	3643	N	ILE	303	60.932	79.198	34.236	1.00	18.30
ATOM	3644	H	ILE	303	61.130	79.742	35.033	1.00	0.00
ATOM	3645	CA	ILE	303	61.795	78.050	33.910	1.00	15.87
ATOM	3646	CB	ILE	303	63.222	78.495	33.439	1.00	15.87
ATOM	3647	CG2	ILE	303	64.032	77.285	33.026	1.00	15.12
ATOM	3648	CG1	ILE	303	63.152	79.437	32.274	1.00	17.94
ATOM	3649	CD1	ILE	303	64.492	79.818	31.610	1.00	18.32
ATOM	3650	C	ILE	303	61.974	77.178	35.169	1.00	14.97
ATOM	3651	O	ILE	303	62.303	77.667	36.237	1.00	15.82
ATOM	3652	N	THR	304	61.735	75.885	35.152	1.00	14.28
ATOM	3653	H	THR	304	61.323	75.533	34.334	1.00	0.00
ATOM	3654	CA	THR	304	61.987	74.999	36.276	1.00	11.17
ATOM	3655	CB	THR	304	60.836	73.999	36.513	1.00	11.73
ATOM	3656	OG1	THR	304	59.791	74.820	37.001	1.00	12.34
ATOM	3657	HG1	THR	304	60.083	75.307	37.786	1.00	0.00
ATOM	3658	CG2	THR	304	61.073	72.873	37.516	1.00	8.94
ATOM	3659	C	THR	304	63.225	74.202	35.970	1.00	12.65
ATOM	3660	O	THR	304	63.321	73.512	34.964	1.00	11.49
ATOM	3661	N	ILE	305	64.266	74.330	36.761	1.00	14.93
ATOM	3662	H	ILE	305	64.238	75.009	37.466	1.00	0.00
ATOM	3663	CA	ILE	305	65.428	73.462	36.601	1.00	15.02
ATOM	3664	CB	ILE	305	66.712	74.396	36.474	1.00	11.43
ATOM	3665	CG2	ILE	305	66.973	75.287	37.652	1.00	9.79
ATOM	3666	CG1	ILE	305	67.906	73.470	36.314	1.00	12.67
ATOM	3667	CD1	ILE	305	67.897	72.824	34.915	1.00	10.15
ATOM	3668	C	ILE	305	65.478	72.415	37.758	1.00	13.96
ATOM	3669	O	ILE	305	65.106	72.677	38.892	1.00	16.32
ATOM	3670	N	PHE	306	65.806	71.157	37.546	1.00	13.27
ATOM	3671	H	PHE	306	66.053	70.905	36.632	1.00	0.00
ATOM	3672	CA	PHE	306	65.796	70.137	38.575	1.00	14.28
ATOM	3673	CB	PHE	306	64.458	69.329	38.388	1.00	12.63
ATOM	3674	CG	PHE	306	64.164	68.354	39.550	1.00	13.60
ATOM	3675	CD1	PHE	306	64.263	66.959	39.348	1.00	11.15
ATOM	3676	CD2	PHE	306	63.861	68.850	40.834	1.00	9.58
ATOM	3677	CE1	PHE	306	64.075	66.085	40.411	1.00	9.70
ATOM	3678	CE2	PHE	306	63.679	67.949	41.885	1.00	10.72
ATOM	3679	CZ	PHE	306	63.786	66.578	41.685	1.00	6.48
ATOM	3680	C	PHE	306	67.065	69.261	38.507	1.00	14.99
ATOM	3681	O	PHE	306	67.288	68.595	37.493	1.00	18.50

83/145

FIGURE 1 (CONT.)

ATOM	3682	N	SER	307	67.934	69.170	39.528	1.00	13.71
ATOM	3683	H	SER	307	67.741	69.599	40.384	1.00	0.00
ATOM	3684	CA	SER	307	69.191	68.424	39.362	1.00	13.70
ATOM	3685	CB	SER	307	70.321	69.352	39.707	1.00	15.42
ATOM	3686	OG	SER	307	70.200	70.599	39.011	1.00	16.93
ATOM	3687	HG	SER	307	70.222	70.439	38.049	1.00	0.00
ATOM	3688	C	SER	307	69.484	67.072	40.029	1.00	16.04
ATOM	3689	O	SER	307	70.614	66.563	40.085	1.00	17.06
ATOM	3690	N	ALA	308	68.407	66.432	40.472	1.00	14.46
ATOM	3691	H	ALA	308	67.562	66.911	40.404	1.00	0.00
ATOM	3692	CA	ALA	308	68.406	65.117	41.078	1.00	13.13
ATOM	3693	CB	ALA	308	67.499	65.192	42.298	1.00	7.67
ATOM	3694	C	ALA	308	67.878	64.104	40.047	1.00	15.64
ATOM	3695	O	ALA	308	66.653	64.097	39.846	1.00	17.74
ATOM	3696	N	PRO	309	68.652	63.307	39.278	1.00	14.64
ATOM	3697	CD	PRO	309	70.089	63.326	39.201	1.00	17.47
ATOM	3698	CA	PRO	309	68.150	62.363	38.305	1.00	17.09
ATOM	3699	CB	PRO	309	69.260	62.195	37.348	1.00	15.02
ATOM	3700	CG	PRO	309	70.428	62.195	38.245	1.00	15.30
ATOM	3701	C	PRO	309	67.747	61.085	39.004	1.00	22.93
ATOM	3702	O	PRO	309	68.229	60.850	40.135	1.00	28.85
ATOM	3703	N	ASN	310	66.897	60.229	38.411	1.00	23.54
ATOM	3704	H	ASN	310	66.597	60.441	37.512	1.00	0.00
ATOM	3705	CA	ASN	310	66.327	59.062	39.093	1.00	19.53
ATOM	3706	CB	ASN	310	67.271	57.894	39.028	1.00	18.91
ATOM	3707	CG	ASN	310	66.507	56.654	39.429	1.00	21.12
ATOM	3708	OD1	ASN	310	65.299	56.529	39.216	1.00	26.53
ATOM	3709	ND2	ASN	310	67.091	55.656	40.051	1.00	23.09
ATOM	3710	HD21	ASN	310	66.454	54.928	40.222	1.00	0.00
ATOM	3711	HD22	ASN	310	68.032	55.681	40.283	1.00	0.00
ATOM	3712	C	ASN	310	65.980	59.364	40.548	1.00	19.31
ATOM	3713	O	ASN	310	66.414	58.774	41.536	1.00	19.31
ATOM	3714	N	TYR	311	65.173	60.407	40.628	1.00	20.90
ATOM	3715	H	TYR	311	64.845	60.760	39.781	1.00	0.00
ATOM	3716	CA	TYR	311	64.705	61.002	41.862	1.00	21.59
ATOM	3717	CB	TYR	311	63.793	62.168	41.533	1.00	22.37
ATOM	3718	CG	TYR	311	63.407	63.000	42.721	1.00	19.95
ATOM	3719	CD1	TYR	311	62.085	63.385	42.857	1.00	21.80
ATOM	3720	CE1	TYR	311	61.683	64.114	43.980	1.00	23.04
ATOM	3721	CD2	TYR	311	64.348	63.336	43.684	1.00	19.85
ATOM	3722	CE2	TYR	311	63.955	64.067	44.806	1.00	21.14
ATOM	3723	CZ	TYR	311	62.629	64.453	44.947	1.00	22.10
ATOM	3724	OH	TYR	311	62.251	65.225	46.032	1.00	25.87
ATOM	3725	HH	TYR	311	61.289	65.155	46.101	1.00	0.00
ATOM	3726	C	TYR	311	63.985	60.057	42.784	1.00	23.03

84/145

FIGURE 1 (CONT.)

ATOM	3727	O	TYR	311	62.878	59.593	42.536	1.00	25.34
ATOM	3728	N	LEU	312	64.648	59.879	43.919	1.00	24.35
ATOM	3729	H	LEU	312	65.436	60.450	44.044	1.00	0.00
ATOM	3730	CA	LEU	312	64.280	58.957	44.994	1.00	24.13
ATOM	3731	CB	LEU	312	62.802	59.012	45.393	1.00	22.50
ATOM	3732	CG	LEU	312	62.044	60.274	45.614	1.00	21.39
ATOM	3733	CD1	LEU	312	60.605	59.922	45.809	1.00	23.61
ATOM	3734	CD2	LEU	312	62.548	60.980	46.803	1.00	20.39
ATOM	3735	C	LEU	312	64.541	57.514	44.581	1.00	23.98
ATOM	3736	O	LEU	312	63.982	56.572	45.140	1.00	25.69
ATOM	3737	N	ASP	313	65.389	57.316	43.571	1.00	24.04
ATOM	3738	H	ASP	313	65.816	58.110	43.197	1.00	0.00
ATOM	3739	CA	ASP	313	65.746	56.002	43.008	1.00	25.47
ATOM	3740	CB	ASP	313	66.373	54.997	44.059	1.00	24.40
ATOM	3741	CG	ASP	313	67.493	55.493	44.977	1.00	24.48
ATOM	3742	OD1	ASP	313	68.443	56.097	44.494	1.00	22.06
ATOM	3743	OD2	ASP	313	67.410	55.285	46.188	1.00	25.28
ATOM	3744	C	ASP	313	64.534	55.292	42.408	1.00	26.13
ATOM	3745	O	ASP	313	64.587	54.142	42.005	1.00	30.76
ATOM	3746	N	VAL	314	63.466	56.046	42.276	1.00	25.66
ATOM	3747	H	VAL	314	63.609	57.002	42.389	1.00	0.00
ATOM	3748	CA	VAL	314	62.138	55.611	41.902	1.00	25.88
ATOM	3749	CB	VAL	314	61.283	55.890	43.163	1.00	25.21
ATOM	3750	CG1	VAL	314	59.822	55.917	42.820	1.00	29.84
ATOM	3751	CG2	VAL	314	61.516	54.794	44.196	1.00	26.41
ATOM	3752	C	VAL	314	61.617	56.307	40.640	1.00	25.00
ATOM	3753	O	VAL	314	61.183	55.660	39.711	1.00	26.42
ATOM	3754	N	TYR	315	61.525	57.637	40.590	1.00	25.47
ATOM	3755	H	TYR	315	61.800	58.133	41.389	1.00	0.00
ATOM	3756	CA	TYR	315	61.125	58.414	39.416	1.00	25.63
ATOM	3757	CB	TYR	315	61.098	59.901	39.720	1.00	27.24
ATOM	3758	CG	TYR	315	60.193	60.519	40.774	1.00	30.56
ATOM	3759	CD1	TYR	315	59.714	59.881	41.917	1.00	32.10
ATOM	3760	CE1	TYR	315	58.867	60.538	42.809	1.00	33.76
ATOM	3761	CD2	TYR	315	59.826	61.831	40.530	1.00	37.13
ATOM	3762	CE2	TYR	315	58.975	62.506	41.421	1.00	40.30
ATOM	3763	CZ	TYR	315	58.501	61.859	42.561	1.00	37.01
ATOM	3764	OH	TYR	315	57.694	62.585	43.419	1.00	36.31
ATOM	3765	HH	TYR	315	57.413	63.396	42.989	1.00	0.00
ATOM	3766	C	TYR	315	62.225	58.189	38.372	1.00	27.40
ATOM	3767	O	TYR	315	63.358	58.500	38.730	1.00	32.40
ATOM	3768	N	ASN	316	62.161	57.750	37.118	1.00	25.08
ATOM	3769	H	ASN	316	61.312	57.440	36.752	1.00	0.00
ATOM	3770	CA	ASN	316	63.444	57.519	36.428	1.00	25.17
ATOM	3771	CB	ASN	316	63.232	56.190	35.739	1.00	26.79

85/145

FIGURE 1 (CONT.)

ATOM	3772	CG	ASN	316	64.312	55.908	34.758	1.00	29.98
ATOM	3773	OD1	ASN	316	65.487	56.147	35.012	1.00	35.47
ATOM	3774	ND2	ASN	316	63.965	55.510	33.552	1.00	32.83
ATOM	3775	HD21	ASN	316	63.038	55.406	33.297	1.00	0.00
ATOM	3776	HD22	ASN	316	64.742	55.390	32.964	1.00	0.00
ATOM	3777	C	ASN	316	63.881	58.684	35.515	1.00	25.21
ATOM	3778	O	ASN	316	64.080	58.633	34.288	1.00	23.89
ATOM	3779	N	ASN	317	64.005	59.826	36.173	1.00	24.64
ATOM	3780	H	ASN	317	63.991	59.808	37.156	1.00	0.00
ATOM	3781	CA	ASN	317	64.201	61.071	35.446	1.00	25.12
ATOM	3782	CB	ASN	317	63.456	62.218	36.169	1.00	27.83
ATOM	3783	CG	ASN	317	64.113	62.544	37.490	1.00	28.75
ATOM	3784	OD1	ASN	317	64.313	61.633	38.284	1.00	27.24
ATOM	3785	ND2	ASN	317	64.565	63.757	37.754	1.00	29.52
ATOM	3786	HD21	ASN	317	64.484	64.445	37.061	1.00	0.00
ATOM	3787	HD22	ASN	317	65.006	63.866	38.624	1.00	0.00
ATOM	3788	C	ASN	317	65.623	61.548	35.166	1.00	24.17
ATOM	3789	O	ASN	317	66.610	61.174	35.819	1.00	24.18
ATOM	3790	N	LYS	318	65.682	62.337	34.109	1.00	18.96
ATOM	3791	H	LYS	318	64.888	62.438	33.542	1.00	0.00
ATOM	3792	CA	LYS	318	66.885	63.047	33.830	1.00	17.86
ATOM	3793	CB	LYS	318	66.855	63.605	32.420	1.00	17.44
ATOM	3794	CG	LYS	318	67.219	62.470	31.513	1.00	18.88
ATOM	3795	CD	LYS	318	67.362	62.936	30.096	1.00	21.37
ATOM	3796	CE	LYS	318	68.160	61.856	29.359	1.00	22.37
ATOM	3797	NZ	LYS	318	68.251	62.162	27.938	1.00	22.60
ATOM	3798	HZ1	LYS	318	67.287	62.231	27.549	1.00	0.00
ATOM	3799	HZ2	LYS	318	68.762	61.395	27.453	1.00	0.00
ATOM	3800	HZ3	LYS	318	68.750	63.062	27.793	1.00	0.00
ATOM	3801	C	LYS	318	66.964	64.207	34.815	1.00	18.82
ATOM	3802	O	LYS	318	65.973	64.597	35.453	1.00	19.70
ATOM	3803	N	ALA	319	68.167	64.717	35.009	1.00	16.81
ATOM	3804	H	ALA	319	68.944	64.221	34.675	1.00	0.00
ATOM	3805	CA	ALA	319	68.313	65.988	35.670	1.00	12.88
ATOM	3806	CB	ALA	319	69.295	65.955	36.747	1.00	14.57
ATOM	3807	C	ALA	319	68.883	66.942	34.657	1.00	16.04
ATOM	3808	O	ALA	319	69.161	66.594	33.494	1.00	13.94
ATOM	3809	N	ALA	320	69.091	68.179	35.093	1.00	17.44
ATOM	3810	H	ALA	320	68.695	68.470	35.943	1.00	0.00
ATOM	3811	CA	ALA	320	69.738	69.120	34.220	1.00	16.48
ATOM	3812	CB	ALA	320	68.732	69.604	33.152	1.00	17.51
ATOM	3813	C	ALA	320	70.268	70.307	34.988	1.00	17.51
ATOM	3814	O	ALA	320	69.780	70.588	36.084	1.00	17.34
ATOM	3815	N	VAL	321	71.315	70.920	34.422	1.00	17.83
ATOM	3816	H	VAL	321	71.729	70.451	33.665	1.00	0.00

FIGURE 1 (CONT.)

ATOM	3817	CA	VAL	321	71.833	72.226	34.809	1.00	17.28
ATOM	3818	CB	VAL	321	73.390	72.343	35.024	1.00	18.81
ATOM	3819	CG1	VAL	321	73.695	71.611	36.293	1.00	19.75
ATOM	3820	CG2	VAL	321	74.239	71.739	33.931	1.00	19.58
ATOM	3821	C	VAL	321	71.520	73.208	33.690	1.00	18.87
ATOM	3822	O	VAL	321	71.438	72.863	32.503	1.00	21.36
ATOM	3823	N	LEU	322	71.368	74.473	34.022	1.00	17.74
ATOM	3824	H	LEU	322	71.485	74.724	34.964	1.00	0.00
ATOM	3825	CA	LEU	322	71.049	75.476	33.048	1.00	17.21
ATOM	3826	CB	LEU	322	69.873	76.122	33.647	1.00	16.44
ATOM	3827	CG	LEU	322	68.953	77.111	33.016	1.00	21.00
ATOM	3828	CD1	LEU	322	67.786	77.356	33.982	1.00	22.70
ATOM	3829	CD2	LEU	322	69.671	78.418	32.760	1.00	25.19
ATOM	3830	C	LEU	322	72.259	76.382	32.843	1.00	20.45
ATOM	3831	O	LEU	322	72.547	77.200	33.696	1.00	22.73
ATOM	3832	N	LYS	323	73.025	76.319	31.755	1.00	23.33
ATOM	3833	H	LYS	323	72.802	75.628	31.100	1.00	0.00
ATOM	3834	CA	LYS	323	74.167	77.199	31.499	1.00	24.45
ATOM	3835	CB	LYS	323	75.215	76.389	30.781	1.00	27.34
ATOM	3836	CG	LYS	323	75.833	75.186	31.557	1.00	28.78
ATOM	3837	CD	LYS	323	76.566	74.422	30.454	1.00	34.23
ATOM	3838	CE	LYS	323	77.572	73.329	30.815	1.00	36.72
ATOM	3839	NZ	LYS	323	78.264	72.919	29.604	1.00	35.30
ATOM	3840	HZ1	LYS	323	77.571	72.586	28.904	1.00	0.00
ATOM	3841	HZ2	LYS	323	78.930	72.151	29.819	1.00	0.00
ATOM	3842	HZ3	LYS	323	78.783	73.727	29.207	1.00	0.00
ATOM	3843	C	LYS	323	73.930	78.507	30.735	1.00	26.44
ATOM	3844	O	LYS	323	73.628	78.519	29.544	1.00	27.95
ATOM	3845	N	TYR	324	73.977	79.670	31.393	1.00	27.42
ATOM	3846	H	TYR	324	74.078	79.621	32.362	1.00	0.00
ATOM	3847	CA	TYR	324	73.801	80.958	30.744	1.00	25.80
ATOM	3848	CB	TYR	324	72.969	81.819	31.625	1.00	23.59
ATOM	3849	CG	TYR	324	72.399	83.023	30.899	1.00	24.11
ATOM	3850	CD1	TYR	324	72.652	84.301	31.367	1.00	27.10
ATOM	3851	CE1	TYR	324	72.068	85.414	30.757	1.00	30.71
ATOM	3852	CD2	TYR	324	71.567	82.852	29.801	1.00	27.19
ATOM	3853	CE2	TYR	324	70.974	83.945	29.169	1.00	30.24
ATOM	3854	CZ	TYR	324	71.228	85.229	29.655	1.00	31.54
ATOM	3855	OH	TYR	324	70.625	86.318	29.046	1.00	32.14
ATOM	3856	HH	TYR	324	70.736	87.109	29.589	1.00	0.00
ATOM	3857	C	TYR	324	75.081	81.728	30.398	1.00	28.35
ATOM	3858	O	TYR	324	75.760	82.229	31.292	1.00	30.60
ATOM	3859	N	GLU	325	75.411	81.921	29.113	1.00	28.11
ATOM	3860	H	GLU	325	74.792	81.517	28.460	1.00	0.00
ATOM	3861	CA	GLU	325	76.561	82.696	28.621	1.00	26.50

87/145

FIGURE 1 (CONT.)

ATOM	3862	CB	GLU	325	77.734	81.781	28.488	1.00	25.00
ATOM	3863	CG	GLU	325	79.061	82.430	28.167	1.00	24.51
ATOM	3864	CD	GLU	325	80.288	81.622	28.553	1.00	25.96
ATOM	3865	OE1	GLU	325	81.347	82.204	28.764	1.00	28.64
ATOM	3866	OE2	GLU	325	80.209	80.410	28.669	1.00	23.60
ATOM	3867	C	GLU	325	76.315	83.384	27.264	1.00	29.68
ATOM	3868	O	GLU	325	75.472	82.942	26.477	1.00	31.58
ATOM	3869	N	ASN	326	77.004	84.479	26.910	1.00	29.43
ATOM	3870	H	ASN	326	77.758	84.730	27.483	1.00	0.00
ATOM	3871	CA	ASN	326	76.856	85.222	25.649	1.00	27.35
ATOM	3872	CB	ASN	326	77.858	84.687	24.601	1.00	28.21
ATOM	3873	CG	ASN	326	79.319	84.515	25.039	1.00	32.70
ATOM	3874	OD1	ASN	326	79.717	84.825	26.144	1.00	37.70
ATOM	3875	ND2	ASN	326	80.309	83.995	24.347	1.00	36.57
ATOM	3876	HD21	ASN	326	80.156	83.665	23.442	1.00	0.00
ATOM	3877	HD22	ASN	326	81.150	83.993	24.837	1.00	0.00
ATOM	3878	C	ASN	326	75.450	85.234	25.037	1.00	26.03
ATOM	3879	O	ASN	326	75.242	84.999	23.846	1.00	26.65
ATOM	3880	N	ASN	327	74.490	85.488	25.932	1.00	23.28
ATOM	3881	H	ASN	327	74.798	85.604	26.849	1.00	0.00
ATOM	3882	CA	ASN	327	73.050	85.630	25.670	1.00	24.87
ATOM	3883	CB	ASN	327	72.856	86.713	24.625	1.00	28.32
ATOM	3884	CG	ASN	327	71.489	87.391	24.657	1.00	34.63
ATOM	3885	OD1	ASN	327	71.093	87.960	25.673	1.00	35.74
ATOM	3886	ND2	ASN	327	70.683	87.393	23.595	1.00	34.60
ATOM	3887	HD21	ASN	327	70.947	86.929	22.784	1.00	0.00
ATOM	3888	HD22	ASN	327	69.858	87.887	23.756	1.00	0.00
ATOM	3889	C	ASN	327	72.240	84.381	25.268	1.00	24.91
ATOM	3890	O	ASN	327	71.083	84.377	24.810	1.00	24.50
ATOM	3891	N	VAL	328	72.876	83.253	25.518	1.00	23.09
ATOM	3892	H	VAL	328	73.776	83.299	25.880	1.00	0.00
ATOM	3893	CA	VAL	328	72.287	81.958	25.229	1.00	22.77
ATOM	3894	CB	VAL	328	73.256	81.144	24.303	1.00	21.00
ATOM	3895	CG1	VAL	328	72.666	79.807	23.973	1.00	18.03
ATOM	3896	CG2	VAL	328	73.523	81.879	22.994	1.00	19.70
ATOM	3897	C	VAL	328	72.093	81.253	26.579	1.00	23.61
ATOM	3898	O	VAL	328	72.824	81.433	27.545	1.00	24.60
ATOM	3899	N	MET	329	71.052	80.464	26.683	1.00	24.83
ATOM	3900	H	MET	329	70.425	80.448	25.929	1.00	0.00
ATOM	3901	CA	MET	329	70.747	79.655	27.834	1.00	25.19
ATOM	3902	CB	MET	329	69.379	79.989	28.347	1.00	28.01
ATOM	3903	CG	MET	329	69.113	79.211	29.599	1.00	32.69
ATOM	3904	SD	MET	329	67.782	79.943	30.571	1.00	39.20
ATOM	3905	CE	MET	329	68.494	81.453	31.169	1.00	36.28
ATOM	3906	C	MET	329	70.750	78.232	27.350	1.00	25.28

FIGURE 1 (CONT.)

ATOM	3907	O	MET	329	69.845	77.816	26.627	1.00	27.67
ATOM	3908	N	ASN	330	71.776	77.469	27.649	1.00	26.19
ATOM	3909	H	ASN	330	72.514	77.846	28.173	1.00	0.00
ATOM	3910	CA	ASN	330	71.805	76.092	27.215	1.00	27.50
ATOM	3911	CB	ASN	330	73.181	75.666	26.730	1.00	28.29
ATOM	3912	CG	ASN	330	73.151	74.301	26.043	1.00	31.11
ATOM	3913	OD1	ASN	330	73.982	73.400	26.217	1.00	33.46
ATOM	3914	ND2	ASN	330	72.165	74.059	25.208	1.00	29.11
ATOM	3915	HD21	ASN	330	72.242	73.182	24.789	1.00	0.00
ATOM	3916	HD22	ASN	330	71.472	74.718	25.043	1.00	0.00
ATOM	3917	C	ASN	330	71.425	75.175	28.355	1.00	28.52
ATOM	3918	O	ASN	330	71.839	75.376	29.497	1.00	30.94
ATOM	3919	N	ILE	331	70.580	74.195	28.078	1.00	26.45
ATOM	3920	H	ILE	331	70.137	74.183	27.210	1.00	0.00
ATOM	3921	CA	ILE	331	70.258	73.183	29.071	1.00	22.75
ATOM	3922	CB	ILE	331	68.795	72.744	28.873	1.00	20.41
ATOM	3923	CG2	ILE	331	68.510	71.436	29.642	1.00	18.06
ATOM	3924	CG1	ILE	331	67.897	73.948	29.184	1.00	18.27
ATOM	3925	CD1	ILE	331	67.948	74.555	30.600	1.00	18.18
ATOM	3926	C	ILE	331	71.220	72.014	28.865	1.00	23.36
ATOM	3927	O	ILE	331	71.410	71.541	27.739	1.00	25.07
ATOM	3928	N	ARG	332	71.851	71.564	29.940	1.00	22.29
ATOM	3929	H	ARG	332	71.790	72.084	30.769	1.00	0.00
ATOM	3930	CA	ARG	332	72.684	70.386	29.886	1.00	22.25
ATOM	3931	CB	ARG	332	74.057	70.732	30.391	1.00	22.75
ATOM	3932	CG	ARG	332	74.951	71.441	29.399	1.00	23.25
ATOM	3933	CD	ARG	332	75.271	70.550	28.200	1.00	25.46
ATOM	3934	NE	ARG	332	75.946	69.272	28.465	1.00	24.91
ATOM	3935	HE	ARG	332	75.399	68.467	28.584	1.00	0.00
ATOM	3936	CZ	ARG	332	77.278	69.146	28.530	1.00	25.28
ATOM	3937	NH1	ARG	332	77.834	67.965	28.656	1.00	26.08
ATOM	3938	HH11	ARG	332	78.830	67.884	28.708	1.00	0.00
ATOM	3939	HH12	ARG	332	77.262	67.145	28.701	1.00	0.00
ATOM	3940	NH2	ARG	332	78.111	70.170	28.523	1.00	29.65
ATOM	3941	HH21	ARG	332	79.096	70.009	28.577	1.00	0.00
ATOM	3942	HH22	ARG	332	77.761	71.106	28.461	1.00	0.00
ATOM	3943	C	ARG	332	72.097	69.252	30.724	1.00	23.10
ATOM	3944	O	ARG	332	72.093	69.274	31.967	1.00	24.40
ATOM	3945	N	GLN	333	71.548	68.230	30.094	1.00	21.63
ATOM	3946	H	GLN	333	71.546	68.224	29.117	1.00	0.00
ATOM	3947	CA	GLN	333	70.980	67.116	30.878	1.00	20.44
ATOM	3948	CB	GLN	333	69.908	66.323	30.111	1.00	16.81
ATOM	3949	CG	GLN	333	68.871	67.280	29.603	1.00	18.88
ATOM	3950	CD	GLN	333	67.712	66.549	29.023	1.00	20.19
ATOM	3951	OE1	GLN	333	67.869	65.670	28.219	1.00	27.23

89/145

FIGURE 1 (CONT.)

ATOM	3952	NE2	GLN	333	66.465	66.729	29.308	1.00	23.12
ATOM	3953	HE21	GLN	333	66.195	67.363	29.996	1.00	0.00
ATOM	3954	HE22	GLN	333	65.894	66.157	28.771	1.00	0.00
ATOM	3955	C	GLN	333	71.960	66.067	31.360	1.00	18.42
ATOM	3956	O	GLN	333	72.952	65.815	30.679	1.00	20.65
ATOM	3957	N	PHE	334	71.714	65.413	32.482	1.00	16.67
ATOM	3958	H	PHE	334	70.944	65.699	33.022	1.00	0.00
ATOM	3959	CA	PHE	334	72.518	64.272	32.868	1.00	14.00
ATOM	3960	CB	PHE	334	73.611	64.715	33.829	1.00	12.14
ATOM	3961	CG	PHE	334	73.250	65.377	35.176	1.00	10.69
ATOM	3962	CD1	PHE	334	72.865	66.711	35.215	1.00	2.88
ATOM	3963	CD2	PHE	334	73.365	64.635	36.376	1.00	10.68
ATOM	3964	CE1	PHE	334	72.606	67.292	36.437	1.00	7.34
ATOM	3965	CE2	PHE	334	73.100	65.228	37.615	1.00	10.68
ATOM	3966	CZ	PHE	334	72.719	66.569	37.637	1.00	10.84
ATOM	3967	C	PHE	334	71.704	63.129	33.488	1.00	17.32
ATOM	3968	O	PHE	334	70.575	63.273	33.972	1.00	18.71
ATOM	3969	N	ASN	335	72.278	61.937	33.448	1.00	19.12
ATOM	3970	H	ASN	335	73.158	61.864	33.037	1.00	0.00
ATOM	3971	CA	ASN	335	71.641	60.766	34.006	1.00	18.40
ATOM	3972	CB	ASN	335	71.775	59.599	33.056	1.00	20.12
ATOM	3973	CG	ASN	335	70.864	59.713	31.848	1.00	19.52
ATOM	3974	OD1	ASN	335	69.968	60.531	31.716	1.00	23.77
ATOM	3975	ND2	ASN	335	71.021	58.920	30.844	1.00	20.14
ATOM	3976	HD21	ASN	335	71.720	58.244	30.827	1.00	0.00
ATOM	3977	HD22	ASN	335	70.376	59.097	30.130	1.00	0.00
ATOM	3978	C	ASN	335	72.191	60.368	35.354	1.00	19.37
ATOM	3979	O	ASN	335	73.194	60.893	35.805	1.00	21.32
ATOM	3980	N	CYS	336	71.504	59.483	36.046	1.00	19.06
ATOM	3981	H	CYS	336	70.680	59.114	35.656	1.00	0.00
ATOM	3982	CA	CYS	336	71.894	59.127	37.385	1.00	18.14
ATOM	3983	CB	CYS	336	70.777	58.290	38.015	1.00	19.33
ATOM	3984	SG	CYS	336	70.713	56.555	37.490	1.00	22.43
ATOM	3985	C	CYS	336	73.206	58.373	37.481	1.00	18.52
ATOM	3986	O	CYS	336	73.627	57.701	36.537	1.00	17.86
ATOM	3987	N	SER	337	73.838	58.459	38.647	1.00	15.39
ATOM	3988	H	SER	337	73.520	59.074	39.326	1.00	0.00
ATOM	3989	CA	SER	337	75.055	57.713	38.876	1.00	15.10
ATOM	3990	CB	SER	337	76.163	58.661	39.231	1.00	13.90
ATOM	3991	OG	SER	337	76.122	59.834	38.422	1.00	16.53
ATOM	3992	HG	SER	337	76.844	60.416	38.691	1.00	0.00
ATOM	3993	C	SER	337	74.859	56.715	40.001	1.00	15.68
ATOM	3994	O	SER	337	74.095	56.988	40.933	1.00	18.01
ATOM	3995	N	PRO	338	75.464	55.524	40.021	1.00	18.06
ATOM	3996	CD	PRO	338	76.415	55.008	39.014	1.00	17.70

90/145

FIGURE 1 (CONT.)

ATOM	3997	CA	PRO	338	75.282	54.558	41.107	1.00	17.20
ATOM	3998	CB	PRO	338	76.168	53.375	40.678	1.00	16.50
ATOM	3999	CG	PRO	338	77.224	53.982	39.779	1.00	17.15
ATOM	4000	C	PRO	338	75.598	55.093	42.508	1.00	16.33
ATOM	4001	O	PRO	338	76.332	56.070	42.685	1.00	17.24
ATOM	4002	N	HIS	339	74.981	54.576	43.545	1.00	12.58
ATOM	4003	H	HIS	339	74.295	53.891	43.391	1.00	0.00
ATOM	4004	CA	HIS	339	75.464	54.932	44.863	1.00	14.70
ATOM	4005	CB	HIS	339	74.684	56.046	45.467	1.00	12.77
ATOM	4006	CG	HIS	339	73.212	55.762	45.492	1.00	12.22
ATOM	4007	CD2	HIS	339	72.349	56.375	44.645	1.00	11.37
ATOM	4008	ND1	HIS	339	72.517	54.951	46.264	1.00	14.02
ATOM	4009	HD1	HIS	339	72.851	54.310	46.933	1.00	0.00
ATOM	4010	CE1	HIS	339	71.255	55.052	45.918	1.00	12.43
ATOM	4011	NE2	HIS	339	71.183	55.916	44.951	1.00	11.50
ATOM	4012	HE2	HIS	339	70.381	56.393	44.664	1.00	0.00
ATOM	4013	C	HIS	339	75.346	53.746	45.780	1.00	15.47
ATOM	4014	O	HIS	339	74.500	52.904	45.467	1.00	17.77
ATOM	4015	N	PRO	340	76.063	53.625	46.901	1.00	14.63
ATOM	4016	CD	PRO	340	77.133	54.509	47.301	1.00	13.76
ATOM	4017	CA	PRO	340	75.832	52.588	47.901	1.00	13.39
ATOM	4018	CB	PRO	340	76.925	52.780	48.878	1.00	13.92
ATOM	4019	CG	PRO	340	77.161	54.244	48.776	1.00	14.72
ATOM	4020	C	PRO	340	74.458	52.643	48.528	1.00	13.52
ATOM	4021	O	PRO	340	73.765	53.670	48.431	1.00	12.06
ATOM	4022	N	TYR	341	74.090	51.478	49.083	1.00	16.61
ATOM	4023	H	TYR	341	74.789	50.827	49.243	1.00	0.00
ATOM	4024	CA	TYR	341	72.762	51.193	49.619	1.00	15.61
ATOM	4025	CB	TYR	341	72.264	49.773	49.234	1.00	15.84
ATOM	4026	CG	TYR	341	70.766	49.479	49.530	1.00	14.17
ATOM	4027	CD1	TYR	341	69.747	50.215	48.943	1.00	11.52
ATOM	4028	CE1	TYR	341	68.422	50.040	49.316	1.00	7.77
ATOM	4029	CD2	TYR	341	70.417	48.530	50.488	1.00	12.93
ATOM	4030	CE2	TYR	341	69.088	48.350	50.848	1.00	12.43
ATOM	4031	CZ	TYR	341	68.096	49.112	50.273	1.00	9.68
ATOM	4032	OH	TYR	341	66.794	48.964	50.711	1.00	10.36
ATOM	4033	HH	TYR	341	66.710	48.107	51.140	1.00	0.00
ATOM	4034	C	TYR	341	72.721	51.299	51.126	1.00	17.92
ATOM	4035	O	TYR	341	73.527	50.785	51.901	1.00	16.80
ATOM	4036	N	TRP	342	71.736	52.112	51.478	1.00	17.70
ATOM	4037	H	TRP	342	71.246	52.605	50.790	1.00	0.00
ATOM	4038	CA	TRP	342	71.406	52.275	52.862	1.00	17.95
ATOM	4039	CB	TRP	342	71.414	53.705	53.217	1.00	16.93
ATOM	4040	CG	TRP	342	72.729	54.274	53.703	1.00	16.28
ATOM	4041	CD2	TRP	342	73.179	54.203	54.991	1.00	17.44

91/145

FIGURE 1 (CONT.)

ATOM	4042	CE2	TRP	342	74.324	54.997	54.910	1.00	20.45
ATOM	4043	CE3	TRP	342	72.807	53.626	56.198	1.00	18.13
ATOM	4044	CD1	TRP	342	73.522	55.019	52.877	1.00	14.49
ATOM	4045	NE1	TRP	342	74.481	55.454	53.644	1.00	19.39
ATOM	4046	HE1	TRP	342	75.212	56.060	53.365	1.00	0.00
ATOM	4047	CZ2	TRP	342	75.114	55.224	56.049	1.00	18.96
ATOM	4048	CZ3	TRP	342	73.598	53.857	57.332	1.00	20.09
ATOM	4049	CH2	TRP	342	74.740	54.651	57.261	1.00	16.19
ATOM	4050	C	TRP	342	70.014	51.723	53.073	1.00	20.15
ATOM	4051	O	TRP	342	69.165	51.936	52.185	1.00	22.55
ATOM	4052	N	LEU	343	69.753	50.948	54.133	1.00	16.44
ATOM	4053	H	LEU	343	70.482	50.711	54.749	1.00	0.00
ATOM	4054	CA	LEU	343	68.370	50.550	54.369	1.00	16.78
ATOM	4055	CB	LEU	343	68.315	49.589	55.552	1.00	17.45
ATOM	4056	CG	LEU	343	68.604	48.128	55.437	1.00	14.00
ATOM	4057	CD1	LEU	343	69.029	47.546	56.766	1.00	11.12
ATOM	4058	CD2	LEU	343	67.373	47.493	54.893	1.00	13.70
ATOM	4059	C	LEU	343	67.472	51.787	54.673	1.00	20.56
ATOM	4060	O	LEU	343	67.974	52.903	54.989	1.00	19.56
ATOM	4061	N	PRO	344	66.125	51.656	54.611	1.00	22.32
ATOM	4062	CD	PRO	344	65.396	50.570	53.945	1.00	23.54
ATOM	4063	CA	PRO	344	65.182	52.700	55.013	1.00	22.57
ATOM	4064	CB	PRO	344	63.845	52.004	54.990	1.00	22.75
ATOM	4065	CG	PRO	344	63.969	51.127	53.775	1.00	22.34
ATOM	4066	C	PRO	344	65.543	53.270	56.357	1.00	24.22
ATOM	4067	O	PRO	344	66.107	52.553	57.179	1.00	24.35
ATOM	4068	N	ASN	345	65.316	54.560	56.559	1.00	26.09
ATOM	4069	H	ASN	345	64.971	55.066	55.787	1.00	0.00
ATOM	4070	CA	ASN	345	65.604	55.303	57.782	1.00	28.48
ATOM	4071	CB	ASN	345	64.452	55.113	58.716	1.00	33.67
ATOM	4072	CG	ASN	345	63.152	55.572	58.093	1.00	39.40
ATOM	4073	OD1	ASN	345	62.936	56.712	57.667	1.00	41.34
ATOM	4074	ND2	ASN	345	62.220	54.650	58.016	1.00	43.82
ATOM	4075	HD21	ASN	345	62.377	53.781	58.432	1.00	0.00
ATOM	4076	HD22	ASN	345	61.414	54.937	57.545	1.00	0.00
ATOM	4077	C	ASN	345	66.914	55.043	58.546	1.00	30.18
ATOM	4078	O	ASN	345	67.054	55.285	59.752	1.00	33.05
ATOM	4079	N	PHE	346	67.934	54.580	57.790	1.00	27.92
ATOM	4080	H	PHE	346	67.743	54.438	56.839	1.00	0.00
ATOM	4081	CA	PHE	346	69.275	54.245	58.260	1.00	22.26
ATOM	4082	CB	PHE	346	69.928	55.458	58.929	1.00	20.92
ATOM	4083	CG	PHE	346	70.142	56.553	57.915	1.00	15.15
ATOM	4084	CD1	PHE	346	71.152	56.414	56.976	1.00	15.16
ATOM	4085	CD2	PHE	346	69.301	57.651	57.911	1.00	16.25
ATOM	4086	CE1	PHE	346	71.343	57.380	56.012	1.00	15.30

92/145

FIGURE 1 (CONT.)

ATOM	4087	CE2	PHE	346	69.483	58.626	56.946	1.00	18.49
ATOM	4088	CZ	PHE	346	70.501	58.484	56.000	1.00	20.86
ATOM	4089	C	PHE	346	69.289	53.078	59.218	1.00	21.21
ATOM	4090	O	PHE	346	70.279	52.804	59.884	1.00	20.07
ATOM	4091	N	MET	347	68.182	52.333	59.200	1.00	19.98
ATOM	4092	H	MET	347	67.507	52.541	58.527	1.00	0.00
ATOM	4093	CA	MET	347	67.997	51.182	60.051	1.00	20.17
ATOM	4094	CB	MET	347	66.791	50.327	59.733	1.00	23.07
ATOM	4095	CG	MET	347	65.365	50.801	59.807	1.00	24.76
ATOM	4096	SD	MET	347	64.392	49.281	59.704	1.00	24.79
ATOM	4097	CE	MET	347	64.531	48.910	57.979	1.00	24.46
ATOM	4098	C	MET	347	69.137	50.220	59.889	1.00	18.69
ATOM	4099	O	MET	347	69.698	50.098	58.792	1.00	19.17
ATOM	4100	N	ASP	348	69.449	49.548	60.981	1.00	17.35
ATOM	4101	H	ASP	348	69.012	49.798	61.816	1.00	0.00
ATOM	4102	CA	ASP	348	70.480	48.539	60.922	1.00	21.38
ATOM	4103	CB	ASP	348	71.255	48.491	62.224	1.00	20.24
ATOM	4104	CG	ASP	348	70.437	48.150	63.431	1.00	22.19
ATOM	4105	OD1	ASP	348	69.851	49.072	63.997	1.00	24.98
ATOM	4106	OD2	ASP	348	70.415	46.975	63.801	1.00	23.32
ATOM	4107	C	ASP	348	69.966	47.143	60.616	1.00	22.36
ATOM	4108	O	ASP	348	68.791	46.830	60.858	1.00	22.23
ATOM	4109	N	VAL	349	70.870	46.254	60.186	1.00	22.02
ATOM	4110	H	VAL	349	71.806	46.535	60.077	1.00	0.00
ATOM	4111	CA	VAL	349	70.412	44.927	59.800	1.00	22.74
ATOM	4112	CB	VAL	349	71.539	44.086	59.091	1.00	23.46
ATOM	4113	CG1	VAL	349	71.819	44.835	57.804	1.00	21.72
ATOM	4114	CG2	VAL	349	72.782	43.863	59.899	1.00	20.58
ATOM	4115	C	VAL	349	69.826	44.085	60.912	1.00	22.01
ATOM	4116	O	VAL	349	69.065	43.166	60.644	1.00	22.35
ATOM	4117	N	PHE	350	70.120	44.403	62.170	1.00	22.52
ATOM	4118	H	PHE	350	70.794	45.097	62.316	1.00	0.00
ATOM	4119	CA	PHE	350	69.517	43.678	63.296	1.00	20.77
ATOM	4120	CB	PHE	350	70.309	43.977	64.599	1.00	19.68
ATOM	4121	CG	PHE	350	71.687	43.332	64.606	1.00	17.12
ATOM	4122	CD1	PHE	350	71.808	41.949	64.540	1.00	15.34
ATOM	4123	CD2	PHE	350	72.824	44.128	64.679	1.00	17.67
ATOM	4124	CE1	PHE	350	73.073	41.355	64.547	1.00	18.03
ATOM	4125	CE2	PHE	350	74.083	43.523	64.686	1.00	17.42
ATOM	4126	CZ	PHE	350	74.213	42.140	64.620	1.00	16.33
ATOM	4127	C	PHE	350	68.050	44.095	63.417	1.00	19.53
ATOM	4128	O	PHE	350	67.169	43.251	63.238	1.00	21.18
ATOM	4129	N	THR	351	67.798	45.404	63.615	1.00	15.59
ATOM	4130	H	THR	351	68.553	45.985	63.818	1.00	0.00
ATOM	4131	CA	THR	351	66.466	46.024	63.622	1.00	14.70

93/145

FIGURE 1 (CONT.)

ATOM	4132	CB	THR	351	66.557	47.549	63.686	1.00	12.86
ATOM	4133	OG1	THR	351	67.311	47.820	64.829	1.00	16.10
ATOM	4134	HG1	THR	351	66.733	47.904	65.597	1.00	0.00
ATOM	4135	CG2	THR	351	65.287	48.284	63.879	1.00	13.58
ATOM	4136	C	THR	351	65.659	45.695	62.368	1.00	17.28
ATOM	4137	O	THR	351	64.429	45.637	62.436	1.00	22.38
ATOM	4138	N	TRP	352	66.307	45.524	61.198	1.00	15.22
ATOM	4139	H	TRP	352	67.250	45.764	61.180	1.00	0.00
ATOM	4140	CA	TRP	352	65.653	45.089	59.956	1.00	15.01
ATOM	4141	CB	TRP	352	66.626	45.269	58.776	1.00	14.13
ATOM	4142	CG	TRP	352	66.155	44.935	57.349	1.00	10.89
ATOM	4143	CD2	TRP	352	66.867	44.170	56.484	1.00	4.33
ATOM	4144	CE2	TRP	352	66.107	44.239	55.329	1.00	5.98
ATOM	4145	CE3	TRP	352	68.039	43.464	56.544	1.00	2.91
ATOM	4146	CD1	TRP	352	65.001	45.448	56.767	1.00	9.30
ATOM	4147	NE1	TRP	352	65.003	44.999	55.535	1.00	8.92
ATOM	4148	HE1	TRP	352	64.254	45.132	54.908	1.00	0.00
ATOM	4149	CZ2	TRP	352	66.553	43.571	54.207	1.00	8.44
ATOM	4150	CZ3	TRP	352	68.487	42.798	55.427	1.00	4.84
ATOM	4151	CH2	TRP	352	67.754	42.847	54.258	1.00	7.67
ATOM	4152	C	TRP	352	65.139	43.645	59.925	1.00	13.50
ATOM	4153	O	TRP	352	63.976	43.337	59.634	1.00	11.96
ATOM	4154	N	SER	353	66.058	42.743	60.245	1.00	15.84
ATOM	4155	H	SER	353	66.937	43.042	60.562	1.00	0.00
ATOM	4156	CA	SER	353	65.793	41.323	60.211	1.00	17.23
ATOM	4157	CB	SER	353	67.083	40.626	59.898	1.00	19.08
ATOM	4158	OG	SER	353	68.056	40.918	60.889	1.00	22.82
ATOM	4159	HG	SER	353	68.819	41.344	60.481	1.00	0.00
ATOM	4160	C	SER	353	65.171	40.689	61.456	1.00	19.96
ATOM	4161	O	SER	353	64.548	39.625	61.340	1.00	20.39
ATOM	4162	N	LEU	354	65.221	41.286	62.665	1.00	21.50
ATOM	4163	H	LEU	354	65.723	42.122	62.726	1.00	0.00
ATOM	4164	CA	LEU	354	64.715	40.644	63.879	1.00	18.85
ATOM	4165	CB	LEU	354	65.228	41.504	65.066	1.00	20.93
ATOM	4166	CG	LEU	354	65.587	40.801	66.421	1.00	24.45
ATOM	4167	CD1	LEU	354	67.082	40.500	66.536	1.00	22.48
ATOM	4168	CD2	LEU	354	65.197	41.713	67.574	1.00	23.69
ATOM	4169	C	LEU	354	63.206	40.318	64.003	1.00	18.69
ATOM	4170	O	LEU	354	62.886	39.166	64.316	1.00	16.92
ATOM	4171	N	PRO	355	62.171	41.128	63.735	1.00	19.76
ATOM	4172	CD	PRO	355	62.240	42.568	63.623	1.00	19.97
ATOM	4173	CA	PRO	355	60.784	40.672	63.550	1.00	20.68
ATOM	4174	CB	PRO	355	60.036	41.933	63.136	1.00	20.98
ATOM	4175	CG	PRO	355	61.142	42.829	62.643	1.00	21.74
ATOM	4176	C	PRO	355	60.530	39.490	62.601	1.00	21.57

94/145

FIGURE 1 (CONT.)

ATOM	4177	O	PRO	355	59.633	38.674	62.813	1.00	23.30
ATOM	4178	N	PHE	356	61.346	39.298	61.572	1.00	22.75
ATOM	4179	H	PHE	356	62.102	39.909	61.459	1.00	0.00
ATOM	4180	CA	PHE	356	61.232	38.133	60.697	1.00	23.52
ATOM	4181	CB	PHE	356	61.774	38.541	59.354	1.00	24.59
ATOM	4182	CG	PHE	356	61.571	37.484	58.299	1.00	25.40
ATOM	4183	CD1	PHE	356	60.277	37.100	57.947	1.00	24.62
ATOM	4184	CD2	PHE	356	62.686	36.925	57.679	1.00	25.81
ATOM	4185	CE1	PHE	356	60.116	36.139	56.946	1.00	27.09
ATOM	4186	CE2	PHE	356	62.499	35.971	56.691	1.00	27.40
ATOM	4187	CZ	PHE	356	61.223	35.571	56.315	1.00	25.41
ATOM	4188	C	PHE	356	61.955	36.886	61.245	1.00	24.71
ATOM	4189	O	PHE	356	61.581	35.729	61.015	1.00	26.29
ATOM	4190	N	VAL	357	63.050	37.079	61.972	1.00	26.15
ATOM	4191	H	VAL	357	63.501	37.949	61.941	1.00	0.00
ATOM	4192	CA	VAL	357	63.650	35.991	62.737	1.00	27.41
ATOM	4193	CB	VAL	357	65.002	36.532	63.304	1.00	28.60
ATOM	4194	CG1	VAL	357	65.578	35.574	64.339	1.00	26.87
ATOM	4195	CG2	VAL	357	65.982	36.719	62.165	1.00	26.28
ATOM	4196	C	VAL	357	62.641	35.569	63.858	1.00	28.05
ATOM	4197	O	VAL	357	62.366	34.406	64.154	1.00	26.26
ATOM	4198	N	GLY	358	62.022	36.530	64.535	1.00	27.50
ATOM	4199	H	GLY	358	62.343	37.436	64.424	1.00	0.00
ATOM	4200	CA	GLY	358	61.005	36.228	65.509	1.00	29.46
ATOM	4201	C	GLY	358	59.889	35.379	64.921	1.00	30.47
ATOM	4202	O	GLY	358	59.485	34.332	65.440	1.00	30.98
ATOM	4203	N	GLU	359	59.433	35.830	63.760	1.00	31.37
ATOM	4204	H	GLU	359	59.780	36.685	63.425	1.00	0.00
ATOM	4205	CA	GLU	359	58.351	35.160	63.058	1.00	29.44
ATOM	4206	CB	GLU	359	58.017	35.967	61.863	1.00	27.90
ATOM	4207	CG	GLU	359	56.910	35.350	61.068	1.00	25.03
ATOM	4208	CD	GLU	359	56.409	36.359	60.105	1.00	26.28
ATOM	4209	OE1	GLU	359	55.252	36.743	60.247	1.00	29.15
ATOM	4210	OE2	GLU	359	57.184	36.758	59.247	1.00	27.05
ATOM	4211	C	GLU	359	58.488	33.722	62.619	1.00	28.39
ATOM	4212	O	GLU	359	57.698	32.854	62.964	1.00	28.95
ATOM	4213	N	LYS	360	59.454	33.474	61.783	1.00	29.66
ATOM	4214	H	LYS	360	60.058	34.201	61.503	1.00	0.00
ATOM	4215	CA	LYS	360	59.620	32.129	61.274	1.00	32.22
ATOM	4216	CB	LYS	360	60.549	32.214	60.081	1.00	31.97
ATOM	4217	CG	LYS	360	59.933	33.059	58.976	1.00	31.76
ATOM	4218	CD	LYS	360	58.850	32.296	58.266	1.00	30.70
ATOM	4219	CE	LYS	360	58.190	33.212	57.265	1.00	33.27
ATOM	4220	NZ	LYS	360	57.419	32.455	56.290	1.00	36.09
ATOM	4221	HZ1	LYS	360	56.634	31.975	56.775	1.00	0.00

95/145

FIGURE 1 (CONT.)

ATOM	4222	HZ2	LYS	360	58.032	31.751	55.833	1.00	0.00
ATOM	4223	HZ3	LYS	360	57.042	33.108	55.574	1.00	0.00
ATOM	4224	C	LYS	360	60.140	31.181	62.352	1.00	32.07
ATOM	4225	O	LYS	360	59.833	29.993	62.304	1.00	33.67
ATOM	4226	N	VAL	361	60.883	31.678	63.364	1.00	32.66
ATOM	4227	H	VAL	361	61.216	32.601	63.285	1.00	0.00
ATOM	4228	CA	VAL	361	61.289	30.896	64.550	1.00	30.72
ATOM	4229	CB	VAL	361	62.279	31.708	65.350	1.00	27.64
ATOM	4230	CG1	VAL	361	62.399	31.351	66.800	1.00	26.98
ATOM	4231	CG2	VAL	361	63.580	31.420	64.670	1.00	26.02
ATOM	4232	C	VAL	361	60.072	30.532	65.391	1.00	31.94
ATOM	4233	O	VAL	361	59.831	29.351	65.612	1.00	34.95
ATOM	4234	N	THR	362	59.251	31.489	65.833	1.00	32.24
ATOM	4235	H	THR	362	59.557	32.418	65.771	1.00	0.00
ATOM	4236	CA	THR	362	57.979	31.219	66.510	1.00	31.58
ATOM	4237	CB	THR	362	57.225	32.535	66.729	1.00	31.93
ATOM	4238	OG1	THR	362	58.068	33.301	67.589	1.00	33.08
ATOM	4239	HG1	THR	362	58.397	34.068	67.101	1.00	0.00
ATOM	4240	CG2	THR	362	55.835	32.376	67.313	1.00	32.64
ATOM	4241	C	THR	362	57.105	30.273	65.691	1.00	31.89
ATOM	4242	O	THR	362	56.702	29.203	66.171	1.00	34.09
ATOM	4243	N	GLU	363	56.861	30.570	64.409	1.00	31.31
ATOM	4244	H	GLU	363	57.226	31.404	64.054	1.00	0.00
ATOM	4245	CA	GLU	363	56.062	29.688	63.543	1.00	29.58
ATOM	4246	CB	GLU	363	55.942	30.135	62.098	1.00	32.45
ATOM	4247	CG	GLU	363	55.131	31.396	61.767	1.00	38.02
ATOM	4248	CD	GLU	363	55.344	31.945	60.342	1.00	41.06
ATOM	4249	OE1	GLU	363	54.820	33.033	60.052	1.00	40.10
ATOM	4250	OE2	GLU	363	56.025	31.294	59.531	1.00	39.79
ATOM	4251	C	GLU	363	56.653	28.307	63.450	1.00	25.77
ATOM	4252	O	GLU	363	55.884	27.366	63.572	1.00	27.98
ATOM	4253	N	MET	364	57.978	28.152	63.341	1.00	21.88
ATOM	4254	H	MET	364	58.531	28.960	63.286	1.00	0.00
ATOM	4255	CA	MET	364	58.629	26.850	63.267	1.00	20.42
ATOM	4256	CB	MET	364	60.150	26.927	63.378	1.00	19.89
ATOM	4257	CG	MET	364	60.673	25.510	63.284	1.00	18.68
ATOM	4258	SD	MET	364	62.440	25.178	63.448	1.00	26.44
ATOM	4259	CE	MET	364	62.475	23.761	64.530	1.00	22.40
ATOM	4260	C	MET	364	58.160	26.012	64.431	1.00	23.53
ATOM	4261	O	MET	364	57.839	24.845	64.291	1.00	26.17
ATOM	4262	N	LEU	365	58.053	26.654	65.583	1.00	24.44
ATOM	4263	H	LEU	365	58.314	27.599	65.615	1.00	0.00
ATOM	4264	CA	LEU	365	57.651	26.003	66.801	1.00	24.41
ATOM	4265	CB	LEU	365	58.184	26.830	67.959	1.00	23.48
ATOM	4266	CG	LEU	365	59.646	26.760	68.160	1.00	19.19

96/145

FIGURE 1 (CONT.)

ATOM	4267	CD1	LEU	365	59.998	27.794	69.159	1.00	21.11
ATOM	4268	CD2	LEU	365	60.055	25.399	68.620	1.00	19.79
ATOM	4269	C	LEU	365	56.150	25.787	66.956	1.00	25.89
ATOM	4270	O	LEU	365	55.752	24.769	67.534	1.00	22.80
ATOM	4271	N	VAL	366	55.295	26.728	66.507	1.00	25.68
ATOM	4272	H	VAL	366	55.646	27.566	66.145	1.00	0.00
ATOM	4273	CA	VAL	366	53.883	26.444	66.602	1.00	26.42
ATOM	4274	CB	VAL	366	52.986	27.668	66.202	1.00	27.47
ATOM	4275	CG1	VAL	366	53.376	28.871	67.037	1.00	26.27
ATOM	4276	CG2	VAL	366	53.115	28.031	64.750	1.00	31.98
ATOM	4277	C	VAL	366	53.677	25.253	65.652	1.00	28.74
ATOM	4278	O	VAL	366	53.191	24.220	66.091	1.00	32.36
ATOM	4279	N	ASN	367	54.191	25.217	64.429	1.00	28.54
ATOM	4280	H	ASN	367	54.559	26.043	64.055	1.00	0.00
ATOM	4281	CA	ASN	367	54.136	24.012	63.601	1.00	30.74
ATOM	4282	CB	ASN	367	54.847	24.291	62.297	1.00	32.99
ATOM	4283	CG	ASN	367	54.032	25.291	61.504	1.00	35.43
ATOM	4284	OD1	ASN	367	53.257	26.114	61.987	1.00	37.16
ATOM	4285	ND2	ASN	367	54.137	25.255	60.206	1.00	37.37
ATOM	4286	HD21	ASN	367	53.586	25.928	59.767	1.00	0.00
ATOM	4287	HD22	ASN	367	54.713	24.609	59.760	1.00	0.00
ATOM	4288	C	ASN	367	54.709	22.721	64.177	1.00	30.03
ATOM	4289	O	ASN	367	54.151	21.641	64.072	1.00	30.48
ATOM	4290	N	VAL	368	55.887	22.770	64.778	1.00	32.11
ATOM	4291	H	VAL	368	56.354	23.631	64.816	1.00	0.00
ATOM	4292	CA	VAL	368	56.490	21.572	65.380	1.00	30.74
ATOM	4293	CB	VAL	368	57.945	21.888	65.752	1.00	25.54
ATOM	4294	CG1	VAL	368	58.601	21.044	66.821	1.00	25.93
ATOM	4295	CG2	VAL	368	58.663	21.545	64.479	1.00	25.45
ATOM	4296	C	VAL	368	55.708	21.063	66.571	1.00	31.98
ATOM	4297	O	VAL	368	55.821	19.883	66.903	1.00	34.28
ATOM	4298	N	LEU	369	54.883	21.875	67.219	1.00	30.89
ATOM	4299	H	LEU	369	54.793	22.819	66.960	1.00	0.00
ATOM	4300	CA	LEU	369	54.054	21.321	68.256	1.00	31.88
ATOM	4301	CB	LEU	369	54.019	22.325	69.404	1.00	28.75
ATOM	4302	CG	LEU	369	55.313	22.910	70.012	1.00	28.06
ATOM	4303	CD1	LEU	369	54.843	23.559	71.296	1.00	26.76
ATOM	4304	CD2	LEU	369	56.418	21.918	70.293	1.00	21.34
ATOM	4305	C	LEU	369	52.673	21.034	67.634	1.00	34.65
ATOM	4306	O	LEU	369	51.619	21.499	68.077	1.00	38.13
ATOM	4307	N	ALA	370	52.783	20.108	66.662	1.00	35.98
ATOM	4308	H	ALA	370	53.669	19.712	66.568	1.00	0.00
ATOM	4309	CA	ALA	370	51.770	19.667	65.694	1.00	36.22
ATOM	4310	CB	ALA	370	51.850	18.135	65.554	1.00	35.48
ATOM	4311	C	ALA	370	50.310	20.040	65.859	1.00	36.80

97/145

FIGURE 1 (CONT.)

ATOM	4312	O	ALA	370	49.949	21.166	65.490	1.00	38.97
------	------	---	-----	-----	--------	--------	--------	------	-------

CALCINEURIN SUBUNIT B COORDINATES

ATOM	Atom									
	Type	Residue #	X	Y	Z	OCC	B			
ATOM	4313	CB	ALA 5	68.996	3.990	78.300	1.00	43.20		
ATOM	4314	C	ALA 5	67.752	4.521	80.411	1.00	39.74		
ATOM	4315	O	ALA 5	66.721	4.569	81.082	1.00	40.79		
ATOM	4316	HT1	ALA 5	66.618	5.263	78.122	1.00	0.00		
ATOM	4317	HT2	ALA 5	65.668	4.153	78.943	1.00	0.00		
ATOM	4318	N	ALA 5	66.506	4.238	78.330	1.00	41.36		
ATOM	4319	HT3	ALA 5	66.360	3.716	77.445	1.00	0.00		
ATOM	4320	CA	ALA 5	67.668	3.763	79.084	1.00	42.01		
ATOM	4321	N	TYR 6	68.839	5.165	80.828	1.00	36.60		
ATOM	4322	H	TYR 6	69.646	5.223	80.283	1.00	0.00		
ATOM	4323	CA	TYR 6	68.818	5.871	82.111	1.00	35.13		
ATOM	4324	CB	TYR 6	70.279	6.251	82.455	1.00	32.03		
ATOM	4325	CG	TYR 6	71.066	4.978	82.586	1.00	26.50		
ATOM	4326	CD1	TYR 6	70.872	4.159	83.688	1.00	25.62		
ATOM	4327	CE1	TYR 6	71.551	2.961	83.769	1.00	28.52		
ATOM	4328	CD2	TYR 6	71.925	4.634	81.561	1.00	26.37		
ATOM	4329	CE2	TYR 6	72.607	3.430	81.637	1.00	28.83		
ATOM	4330	CZ	TYR 6	72.422	2.604	82.739	1.00	28.22		
ATOM	4331	OH	TYR 6	73.172	1.456	82.844	1.00	30.10		
ATOM	4332	HH	TYR 6	74.065	1.601	82.505	1.00	0.00		
ATOM	4333	C	TYR 6	67.891	7.101	82.151	1.00	32.47		
ATOM	4334	O	TYR 6	67.321	7.471	81.100	1.00	31.50		
ATOM	4335	N	PRO 7	67.662	7.710	83.321	1.00	30.37		
ATOM	4336	CD	PRO 7	68.018	7.204	84.631	1.00	27.64		
ATOM	4337	CA	PRO 7	66.867	8.931	83.429	1.00	30.75		
ATOM	4338	CB	PRO 7	66.845	9.236	84.903	1.00	29.60		
ATOM	4339	CG	PRO 7	66.948	7.851	85.476	1.00	30.15		
ATOM	4340	C	PRO 7	67.430	10.072	82.599	1.00	30.04		
ATOM	4341	O	PRO 7	68.551	9.995	82.073	1.00	32.39		
ATOM	4342	N	LEU 8	66.678	11.131	82.395	1.00	28.53		
ATOM	4343	H	LEU 8	65.747	11.108	82.710	1.00	0.00		
ATOM	4344	CA	LEU 8	67.231	12.265	81.676	1.00	27.91		
ATOM	4345	CB	LEU 8	66.347	12.612	80.505	1.00	30.34		
ATOM	4346	CG	LEU 8	65.873	11.530	79.554	1.00	32.13		
ATOM	4347	CD1	LEU 8	64.748	12.129	78.747	1.00	31.79		
ATOM	4348	CD2	LEU 8	67.011	11.011	78.669	1.00	32.09		
ATOM	4349	C	LEU 8	67.292	13.459	82.607	1.00	26.46		
ATOM	4350	O	LEU 8	66.285	13.681	83.271	1.00	28.90		
ATOM	4351	N	GLU 9	68.352	14.227	82.805	1.00	24.83		

FIGURE 1 (CONT.)

ATOM	4352	H	GLU	9	69.210	13.979	82.407	1.00	0.00
ATOM	4353	CA	GLU	9	68.204	15.449	83.579	1.00	25.20
ATOM	4354	CB	GLU	9	69.413	15.727	84.527	1.00	27.85
ATOM	4355	CG	GLU	9	70.848	15.880	83.980	1.00	32.21
ATOM	4356	CD	GLU	9	71.375	17.231	83.462	1.00	33.39
ATOM	4357	OE1	GLU	9	72.445	17.228	82.826	1.00	33.56
ATOM	4358	OE2	GLU	9	70.754	18.271	83.699	1.00	33.78
ATOM	4359	C	GLU	9	68.085	16.586	82.570	1.00	25.53
ATOM	4360	O	GLU	9	68.608	16.510	81.452	1.00	22.83
ATOM	4361	N	MET	10	67.355	17.638	82.985	1.00	25.63
ATOM	4362	H	MET	10	66.913	17.531	83.857	1.00	0.00
ATOM	4363	CA	MET	10	67.072	18.850	82.195	1.00	22.21
ATOM	4364	CB	MET	10	65.962	18.576	81.153	1.00	20.45
ATOM	4365	CG	MET	10	64.683	17.900	81.644	1.00	18.85
ATOM	4366	SD	MET	10	63.637	17.395	80.263	1.00	23.92
ATOM	4367	CE	MET	10	64.421	15.895	79.759	1.00	19.95
ATOM	4368	C	MET	10	66.611	20.034	83.037	1.00	21.86
ATOM	4369	O	MET	10	66.121	19.892	84.163	1.00	22.80
ATOM	4370	N	CYS	11	66.659	21.232	82.498	1.00	21.34
ATOM	4371	H	CYS	11	67.032	21.331	81.596	1.00	0.00
ATOM	4372	CA	CYS	11	66.130	22.399	83.210	1.00	20.10
ATOM	4373	CB	CYS	11	67.313	23.297	83.616	1.00	20.74
ATOM	4374	SG	CYS	11	66.808	24.872	84.345	1.00	22.79
ATOM	4375	C	CYS	11	65.117	23.174	82.356	1.00	18.00
ATOM	4376	O	CYS	11	65.406	23.571	81.242	1.00	17.85
ATOM	4377	N	SER	12	63.914	23.453	82.797	1.00	18.58
ATOM	4378	H	SER	12	63.704	23.255	83.738	1.00	0.00
ATOM	4379	CA	SER	12	62.912	24.124	81.966	1.00	19.13
ATOM	4380	CB	SER	12	62.112	23.169	81.167	1.00	19.31
ATOM	4381	OG	SER	12	61.608	22.112	81.995	1.00	20.90
ATOM	4382	HG	SER	12	61.163	22.351	82.830	1.00	0.00
ATOM	4383	C	SER	12	61.861	24.912	82.718	1.00	21.25
ATOM	4384	O	SER	12	61.743	24.772	83.921	1.00	23.67
ATOM	4385	N	HIS	13	60.998	25.708	82.078	1.00	22.81
ATOM	4386	H	HIS	13	61.113	25.793	81.114	1.00	0.00
ATOM	4387	CA	HIS	13	59.879	26.365	82.760	1.00	20.37
ATOM	4388	CB	HIS	13	59.517	27.589	82.042	1.00	19.47
ATOM	4389	CG	HIS	13	60.525	28.699	82.196	1.00	20.32
ATOM	4390	CD2	HIS	13	61.291	29.195	81.170	1.00	19.77
ATOM	4391	ND1	HIS	13	60.783	29.430	83.274	1.00	20.82
ATOM	4392	HD1	HIS	13	60.411	29.335	84.180	1.00	0.00
ATOM	4393	CE1	HIS	13	61.660	30.357	82.954	1.00	18.39
ATOM	4394	NE2	HIS	13	61.951	30.194	81.688	1.00	19.37
ATOM	4395	HE2	HIS	13	62.549	30.804	81.193	1.00	0.00
ATOM	4396	C	HIS	13	58.610	25.524	82.868	1.00	21.27

99/145

FIGURE 1 (CONT.)

ATOM	4397	O	HIS	13	57.573	25.933	83.381	1.00	23.84
ATOM	4398	N	PHE	14	58.667	24.308	82.371	1.00	20.73
ATOM	4399	H	PHE	14	59.536	23.905	82.200	1.00	0.00
ATOM	4400	CA	PHE	14	57.495	23.461	82.292	1.00	21.21
ATOM	4401	CB	PHE	14	57.585	22.520	81.042	1.00	19.24
ATOM	4402	CG	PHE	14	57.839	23.228	79.712	1.00	18.18
ATOM	4403	CD1	PHE	14	58.947	22.858	78.936	1.00	19.31
ATOM	4404	CD2	PHE	14	57.045	24.310	79.299	1.00	16.17
ATOM	4405	CE1	PHE	14	59.245	23.592	77.769	1.00	19.07
ATOM	4406	CE2	PHE	14	57.350	25.026	78.146	1.00	8.90
ATOM	4407	CZ	PHE	14	58.439	24.676	77.390	1.00	14.37
ATOM	4408	C	PHE	14	57.247	22.598	83.529	1.00	22.84
ATOM	4409	O	PHE	14	58.135	22.050	84.191	1.00	21.43
ATOM	4410	N	ASP	15	55.958	22.477	83.805	1.00	24.44
ATOM	4411	H	ASP	15	55.343	23.099	83.374	1.00	0.00
ATOM	4412	CA	ASP	15	55.495	21.517	84.786	1.00	25.80
ATOM	4413	CB	ASP	15	54.174	22.042	85.359	1.00	25.64
ATOM	4414	CG	ASP	15	52.939	22.084	84.464	1.00	30.17
ATOM	4415	OD1	ASP	15	52.643	21.102	83.775	1.00	33.16
ATOM	4416	OD2	ASP	15	52.232	23.097	84.486	1.00	31.52
ATOM	4417	C	ASP	15	55.342	20.120	84.158	1.00	24.87
ATOM	4418	O	ASP	15	55.504	19.960	82.953	1.00	27.40
ATOM	4419	N	ALA	16	54.914	19.082	84.865	1.00	27.40
ATOM	4420	H	ALA	16	54.813	19.226	85.828	1.00	0.00
ATOM	4421	CA	ALA	16	54.759	17.716	84.338	1.00	25.44
ATOM	4422	CB	ALA	16	54.488	16.782	85.461	1.00	27.16
ATOM	4423	C	ALA	16	53.724	17.412	83.278	1.00	26.54
ATOM	4424	O	ALA	16	53.877	16.410	82.580	1.00	27.26
ATOM	4425	N	ASP	17	52.640	18.183	83.100	1.00	27.46
ATOM	4426	H	ASP	17	52.336	18.733	83.846	1.00	0.00
ATOM	4427	CA	ASP	17	51.791	17.989	81.901	1.00	29.39
ATOM	4428	CB	ASP	17	50.487	18.742	81.835	1.00	33.94
ATOM	4429	CG	ASP	17	49.555	18.585	83.005	1.00	38.23
ATOM	4430	OD1	ASP	17	49.450	17.485	83.587	1.00	37.82
ATOM	4431	OD2	ASP	17	48.937	19.612	83.289	1.00	40.00
ATOM	4432	C	ASP	17	52.468	18.540	80.654	1.00	28.81
ATOM	4433	O	ASP	17	52.475	17.909	79.587	1.00	26.82
ATOM	4434	N	GLU	18	53.089	19.727	80.860	1.00	25.40
ATOM	4435	H	GLU	18	53.020	20.126	81.745	1.00	0.00
ATOM	4436	CA	GLU	18	53.802	20.411	79.783	1.00	22.90
ATOM	4437	CB	GLU	18	54.403	21.701	80.171	1.00	20.45
ATOM	4438	CG	GLU	18	53.327	22.510	80.807	1.00	23.40
ATOM	4439	CD	GLU	18	53.580	23.991	80.803	1.00	27.53
ATOM	4440	OE1	GLU	18	52.814	24.682	80.141	1.00	29.77
ATOM	4441	OE2	GLU	18	54.527	24.456	81.442	1.00	31.72

100/145

FIGURE 1 (CONT.)

ATOM	4442	C	GLU	18	54.932	19.573	79.301	1.00	22.97
ATOM	4443	O	GLU	18	55.052	19.417	78.094	1.00	25.32
ATOM	4444	N	ILE	19	55.704	18.938	80.196	1.00	22.77
ATOM	4445	H	ILE	19	55.631	19.158	81.148	1.00	0.00
ATOM	4446	CA	ILE	19	56.737	18.044	79.704	1.00	20.13
ATOM	4447	CB	ILE	19	57.718	17.616	80.809	1.00	17.46
ATOM	4448	CG2	ILE	19	58.753	16.592	80.315	1.00	12.45
ATOM	4449	CG1	ILE	19	58.413	18.866	81.270	1.00	14.53
ATOM	4450	CD1	ILE	19	59.419	18.623	82.367	1.00	14.67
ATOM	4451	C	ILE	19	56.087	16.834	79.121	1.00	21.16
ATOM	4452	O	ILE	19	56.491	16.416	78.058	1.00	25.31
ATOM	4453	N	ALA	20	55.050	16.247	79.678	1.00	25.11
ATOM	4454	H	ALA	20	54.704	16.581	80.530	1.00	0.00
ATOM	4455	CA	ALA	20	54.464	15.046	79.084	1.00	28.76
ATOM	4456	CB	ALA	20	53.342	14.610	80.026	1.00	26.76
ATOM	4457	C	ALA	20	53.940	15.208	77.629	1.00	31.53
ATOM	4458	O	ALA	20	54.259	14.483	76.664	1.00	29.66
ATOM	4459	N	ARG	21	53.174	16.286	77.452	1.00	33.34
ATOM	4460	H	ARG	21	53.024	16.870	78.214	1.00	0.00
ATOM	4461	CA	ARG	21	52.546	16.561	76.171	1.00	34.72
ATOM	4462	CB	ARG	21	51.484	17.625	76.382	1.00	37.21
ATOM	4463	CG	ARG	21	50.508	17.344	77.576	1.00	42.09
ATOM	4464	CD	ARG	21	49.773	15.990	77.888	1.00	44.07
ATOM	4465	NE	ARG	21	49.126	16.029	79.210	1.00	43.55
ATOM	4466	HE	ARG	21	49.431	15.387	79.884	1.00	0.00
ATOM	4467	CZ	ARG	21	48.130	16.891	79.565	1.00	40.96
ATOM	4468	NH1	ARG	21	47.607	16.877	80.795	1.00	39.06
ATOM	4469	HH11	ARG	21	47.945	16.220	81.470	1.00	0.00
ATOM	4470	HH12	ARG	21	46.874	17.511	81.038	1.00	0.00
ATOM	4471	NH2	ARG	21	47.585	17.757	78.723	1.00	39.24
ATOM	4472	HH21	ARG	21	47.897	17.806	77.775	1.00	0.00
ATOM	4473	HH22	ARG	21	46.857	18.363	79.042	1.00	0.00
ATOM	4474	C	ARG	21	53.578	16.975	75.137	1.00	34.10
ATOM	4475	O	ARG	21	53.572	16.540	73.982	1.00	36.49
ATOM	4476	N	LEU	22	54.592	17.689	75.594	1.00	32.79
ATOM	4477	H	LEU	22	54.554	18.021	76.518	1.00	0.00
ATOM	4478	CA	LEU	22	55.742	18.014	74.753	1.00	31.82
ATOM	4479	CB	LEU	22	56.576	19.022	75.547	1.00	31.09
ATOM	4480	CG	LEU	22	57.371	20.172	74.976	1.00	30.54
ATOM	4481	CD1	LEU	22	56.600	21.072	74.038	1.00	25.60
ATOM	4482	CD2	LEU	22	57.751	20.993	76.155	1.00	25.45
ATOM	4483	C	LEU	22	56.505	16.724	74.404	1.00	31.42
ATOM	4484	O	LEU	22	57.049	16.559	73.309	1.00	34.16
ATOM	4485	N	GLY	23	56.508	15.713	75.266	1.00	30.31
ATOM	4486	H	GLY	23	56.151	15.866	76.166	1.00	0.00

101/145

FIGURE 1 (CONT.)

ATOM	4487	CA	GLY	23	57.120	14.426	74.949	1.00	30.03
ATOM	4488	C	GLY	23	56.283	13.631	73.940	1.00	31.87
ATOM	4489	O	GLY	23	56.802	12.832	73.149	1.00	33.29
ATOM	4490	N	ALA	24	54.951	13.828	73.931	1.00	31.23
ATOM	4491	H	ALA	24	54.570	14.353	74.665	1.00	0.00
ATOM	4492	CA	ALA	24	54.059	13.195	72.941	1.00	28.78
ATOM	4493	CB	ALA	24	52.620	13.561	73.295	1.00	28.27
ATOM	4494	C	ALA	24	54.380	13.632	71.493	1.00	28.51
ATOM	4495	O	ALA	24	54.628	12.821	70.568	1.00	27.58
ATOM	4496	N	ARG	25	54.457	14.971	71.328	1.00	24.88
ATOM	4497	H	ARG	25	54.180	15.536	72.083	1.00	0.00
ATOM	4498	CA	ARG	25	54.969	15.532	70.078	1.00	22.10
ATOM	4499	CB	ARG	25	55.001	17.023	70.186	1.00	16.85
ATOM	4500	CG	ARG	25	53.679	17.556	70.634	1.00	17.34
ATOM	4501	CD	ARG	25	53.907	18.813	71.436	1.00	16.25
ATOM	4502	NE	ARG	25	52.799	19.693	71.198	1.00	20.00
ATOM	4503	HE	ARG	25	52.500	19.811	70.272	1.00	0.00
ATOM	4504	CZ	ARG	25	52.131	20.359	72.139	1.00	25.33
ATOM	4505	NH1	ARG	25	51.151	21.166	71.710	1.00	25.36
ATOM	4506	HH11	ARG	25	50.942	21.226	70.734	1.00	0.00
ATOM	4507	HH12	ARG	25	50.601	21.674	72.372	1.00	0.00
ATOM	4508	NH2	ARG	25	52.374	20.245	73.465	1.00	27.50
ATOM	4509	HH21	ARG	25	53.101	19.639	73.785	1.00	0.00
ATOM	4510	HH22	ARG	25	51.836	20.774	74.121	1.00	0.00
ATOM	4511	C	ARG	25	56.392	14.997	69.779	1.00	23.93
ATOM	4512	O	ARG	25	56.583	14.399	68.724	1.00	25.12
ATOM	4513	N	PHE	26	57.425	15.031	70.644	1.00	26.26
ATOM	4514	H	PHE	26	57.287	15.482	71.506	1.00	0.00
ATOM	4515	CA	PHE	26	58.765	14.508	70.296	1.00	27.68
ATOM	4516	CB	PHE	26	59.687	14.541	71.498	1.00	27.32
ATOM	4517	CG	PHE	26	61.142	14.205	71.185	1.00	24.72
ATOM	4518	CD1	PHE	26	62.020	15.232	70.805	1.00	24.07
ATOM	4519	CD2	PHE	26	61.617	12.886	71.279	1.00	23.51
ATOM	4520	CE1	PHE	26	63.368	14.950	70.518	1.00	21.75
ATOM	4521	CE2	PHE	26	62.959	12.620	70.991	1.00	21.50
ATOM	4522	CZ	PHE	26	63.838	13.646	70.610	1.00	18.22
ATOM	4523	C	PHE	26	58.782	13.085	69.769	1.00	29.91
ATOM	4524	O	PHE	26	59.440	12.738	68.784	1.00	29.09
ATOM	4525	N	ALA	27	58.017	12.248	70.469	1.00	34.66
ATOM	4526	H	ALA	27	57.592	12.567	71.294	1.00	0.00
ATOM	4527	CA	ALA	27	57.798	10.865	70.034	1.00	37.38
ATOM	4528	CB	ALA	27	57.023	10.092	71.128	1.00	34.12
ATOM	4529	C	ALA	27	57.033	10.817	68.688	1.00	38.26
ATOM	4530	O	ALA	27	57.488	10.061	67.818	1.00	38.75
ATOM	4531	N	LYS	28	55.990	11.643	68.388	1.00	37.68

102/145

FIGURE 1 (CONT.)

ATOM	4532	H	LYS	28	55.680	12.266	69.076	1.00	0.00
ATOM	4533	CA	LYS	28	55.353	11.623	67.046	1.00	37.22
ATOM	4534	CB	LYS	28	54.191	12.618	66.904	1.00	36.44
ATOM	4535	CG	LYS	28	52.900	12.336	67.687	1.00	36.78
ATOM	4536	CD	LYS	28	52.030	13.587	67.836	1.00	35.42
ATOM	4537	CE	LYS	28	51.016	13.576	69.004	1.00	34.61
ATOM	4538	NZ	LYS	28	50.402	14.899	69.149	1.00	28.68
ATOM	4539	HZ1	LYS	28	49.693	14.860	69.909	1.00	0.00
ATOM	4540	HZ2	LYS	28	49.930	15.152	68.257	1.00	0.00
ATOM	4541	HZ3	LYS	28	51.122	15.611	69.379	1.00	0.00
ATOM	4542	C	LYS	28	56.331	11.966	65.925	1.00	38.00
ATOM	4543	O	LYS	28	56.240	11.494	64.796	1.00	40.42
ATOM	4544	N	LEU	29	57.318	12.781	66.261	1.00	38.23
ATOM	4545	H	LEU	29	57.290	13.164	67.164	1.00	0.00
ATOM	4546	CA	LEU	29	58.371	13.179	65.348	1.00	38.73
ATOM	4547	CB	LEU	29	58.956	14.536	65.726	1.00	37.72
ATOM	4548	CG	LEU	29	58.235	15.868	65.747	1.00	35.83
ATOM	4549	CD1	LEU	29	58.906	16.782	66.772	1.00	35.68
ATOM	4550	CD2	LEU	29	58.271	16.484	64.373	1.00	33.58
ATOM	4551	C	LEU	29	59.574	12.250	65.244	1.00	40.44
ATOM	4552	O	LEU	29	60.290	12.311	64.244	1.00	42.13
ATOM	4553	N	ASP	30	59.926	11.433	66.241	1.00	42.58
ATOM	4554	H	ASP	30	59.384	11.435	67.060	1.00	0.00
ATOM	4555	CA	ASP	30	61.185	10.651	66.185	1.00	42.30
ATOM	4556	CB	ASP	30	61.405	9.946	67.540	1.00	43.54
ATOM	4557	CG	ASP	30	62.812	9.482	67.936	1.00	44.15
ATOM	4558	OD1	ASP	30	62.936	8.960	69.053	1.00	44.88
ATOM	4559	OD2	ASP	30	63.774	9.624	67.171	1.00	43.78
ATOM	4560	C	ASP	30	61.403	9.623	65.076	1.00	41.27
ATOM	4561	O	ASP	30	62.575	9.342	64.812	1.00	41.73
ATOM	4562	N	LEU	31	60.381	9.048	64.397	1.00	39.76
ATOM	4563	H	LEU	31	59.489	9.303	64.708	1.00	0.00
ATOM	4564	CA	LEU	31	60.487	8.107	63.243	1.00	36.87
ATOM	4565	CB	LEU	31	60.409	8.876	61.929	1.00	33.02
ATOM	4566	CG	LEU	31	59.229	9.805	61.651	1.00	30.30
ATOM	4567	CD1	LEU	31	59.542	10.513	60.367	1.00	27.67
ATOM	4568	CD2	LEU	31	57.890	9.069	61.548	1.00	30.35
ATOM	4569	C	LEU	31	61.679	7.141	63.111	1.00	36.93
ATOM	4570	O	LEU	31	61.462	5.954	62.946	1.00	38.62
ATOM	4571	N	ASP	32	62.955	7.481	63.139	1.00	36.31
ATOM	4572	H	ASP	32	63.184	8.429	63.146	1.00	0.00
ATOM	4573	CA	ASP	32	63.975	6.453	63.287	1.00	39.61
ATOM	4574	CB	ASP	32	65.355	7.007	62.836	1.00	41.25
ATOM	4575	CG	ASP	32	65.512	7.129	61.301	1.00	45.97
ATOM	4576	OD1	ASP	32	64.963	8.080	60.706	1.00	47.73

103/145

FIGURE 1 (CONT.)

ATOM	4577	OD2	ASP	32	66.186	6.269	60.702	1.00	44.58
ATOM	4578	C	ASP	32	64.048	5.950	64.750	1.00	41.47
ATOM	4579	O	ASP	32	64.851	5.091	65.123	1.00	42.13
ATOM	4580	N	ASN	33	63.213	6.448	65.671	1.00	42.53
ATOM	4581	H	ASN	33	62.543	7.091	65.364	1.00	0.00
ATOM	4582	CA	ASN	33	63.236	6.130	67.111	1.00	42.93
ATOM	4583	CB	ASN	33	62.403	4.893	67.366	1.00	42.09
ATOM	4584	CG	ASN	33	60.983	5.238	66.960	1.00	43.57
ATOM	4585	OD1	ASN	33	60.641	6.390	66.680	1.00	43.22
ATOM	4586	ND2	ASN	33	60.075	4.304	66.810	1.00	43.38
ATOM	4587	HD21	ASN	33	60.321	3.372	66.936	1.00	0.00
ATOM	4588	HD22	ASN	33	59.201	4.657	66.555	1.00	0.00
ATOM	4589	C	ASN	33	64.569	5.983	67.823	1.00	43.78
ATOM	4590	O	ASN	33	64.752	5.368	68.880	1.00	45.36
ATOM	4591	N	SER	34	65.475	6.789	67.272	1.00	44.51
ATOM	4592	H	SER	34	65.227	7.281	66.463	1.00	0.00
ATOM	4593	CA	SER	34	66.853	6.941	67.757	1.00	44.38
ATOM	4594	CB	SER	34	67.671	7.741	66.746	1.00	45.95
ATOM	4595	OG	SER	34	66.852	8.737	66.109	1.00	46.88
ATOM	4596	HG	SER	34	66.714	9.521	66.662	1.00	0.00
ATOM	4597	C	SER	34	66.979	7.644	69.097	1.00	42.56
ATOM	4598	O	SER	34	68.050	7.729	69.714	1.00	42.02
ATOM	4599	N	GLY	35	65.847	8.199	69.538	1.00	39.70
ATOM	4600	H	GLY	35	65.011	7.996	69.078	1.00	0.00
ATOM	4601	CA	GLY	35	65.850	8.998	70.742	1.00	38.72
ATOM	4602	C	GLY	35	66.148	10.399	70.278	1.00	38.78
ATOM	4603	O	GLY	35	65.267	11.241	70.328	1.00	38.52
ATOM	4604	N	SER	36	67.359	10.679	69.756	1.00	37.34
ATOM	4605	H	SER	36	68.051	9.988	69.819	1.00	0.00
ATOM	4606	CA	SER	36	67.611	11.971	69.129	1.00	33.09
ATOM	4607	CB	SER	36	68.969	12.027	68.564	1.00	32.13
ATOM	4608	OG	SER	36	69.912	12.565	69.472	1.00	33.95
ATOM	4609	HG	SER	36	69.963	13.526	69.386	1.00	0.00
ATOM	4610	C	SER	36	66.653	12.227	67.988	1.00	33.28
ATOM	4611	O	SER	36	66.100	11.269	67.472	1.00	36.15
ATOM	4612	N	LEU	37	66.380	13.471	67.603	1.00	33.98
ATOM	4613	H	LEU	37	66.635	14.189	68.217	1.00	0.00
ATOM	4614	CA	LEU	37	65.519	13.861	66.476	1.00	31.74
ATOM	4615	CB	LEU	37	64.579	14.905	67.038	1.00	30.55
ATOM	4616	CG	LEU	37	63.206	15.137	66.562	1.00	29.82
ATOM	4617	CD1	LEU	37	62.397	13.891	66.759	1.00	32.01
ATOM	4618	CD2	LEU	37	62.573	16.218	67.398	1.00	31.36
ATOM	4619	C	LEU	37	66.347	14.405	65.301	1.00	32.42
ATOM	4620	O	LEU	37	66.976	15.461	65.371	1.00	30.47
ATOM	4621	N	GLY	38	66.429	13.696	64.175	1.00	37.35

104/145

FIGURE 1 (CONT.)

ATOM	4622	H	GLY	38	65.894	12.874	64.157	1.00	0.00
ATOM	4623	CA	GLY	38	67.269	14.061	62.995	1.00	37.14
ATOM	4624	C	GLY	38	66.775	15.204	62.106	1.00	37.17
ATOM	4625	O	GLY	38	65.563	15.430	62.038	1.00	39.62
ATOM	4626	N	VAL	39	67.642	15.934	61.383	1.00	35.67
ATOM	4627	H	VAL	39	68.591	15.799	61.578	1.00	0.00
ATOM	4628	CA	VAL	39	67.209	17.033	60.480	1.00	35.70
ATOM	4629	CB	VAL	39	68.392	17.525	59.588	1.00	36.97
ATOM	4630	CG1	VAL	39	67.933	18.850	58.978	1.00	36.00
ATOM	4631	CG2	VAL	39	69.722	17.650	60.328	1.00	36.41
ATOM	4632	C	VAL	39	66.037	16.725	59.501	1.00	36.52
ATOM	4633	O	VAL	39	65.116	17.515	59.220	1.00	33.21
ATOM	4634	N	GLY	40	66.158	15.496	58.944	1.00	38.25
ATOM	4635	H	GLY	40	66.985	15.014	59.131	1.00	0.00
ATOM	4636	CA	GLY	40	65.171	14.910	58.037	1.00	37.84
ATOM	4637	C	GLY	40	63.731	15.020	58.555	1.00	37.95
ATOM	4638	O	GLY	40	62.882	15.643	57.922	1.00	39.33
ATOM	4639	N	GLU	41	63.477	14.523	59.770	1.00	38.27
ATOM	4640	H	GLU	41	64.241	14.224	60.300	1.00	0.00
ATOM	4641	CA	GLU	41	62.140	14.479	60.394	1.00	37.37
ATOM	4642	CB	GLU	41	62.206	13.756	61.714	1.00	40.29
ATOM	4643	CG	GLU	41	62.421	12.263	61.445	1.00	42.63
ATOM	4644	CD	GLU	41	63.051	11.431	62.557	1.00	44.09
ATOM	4645	OE1	GLU	41	63.188	11.893	63.690	1.00	44.47
ATOM	4646	OE2	GLU	41	63.407	10.288	62.275	1.00	44.86
ATOM	4647	C	GLU	41	61.520	15.823	60.644	1.00	35.58
ATOM	4648	O	GLU	41	60.311	16.021	60.623	1.00	35.78
ATOM	4649	N	PHE	42	62.405	16.777	60.904	1.00	36.39
ATOM	4650	H	PHE	42	63.335	16.526	61.061	1.00	0.00
ATOM	4651	CA	PHE	42	61.985	18.169	61.032	1.00	35.52
ATOM	4652	CB	PHE	42	63.214	19.013	61.495	1.00	34.46
ATOM	4653	CG	PHE	42	63.469	19.084	63.010	1.00	33.27
ATOM	4654	CD1	PHE	42	62.569	19.771	63.852	1.00	33.16
ATOM	4655	CD2	PHE	42	64.634	18.537	63.554	1.00	32.67
ATOM	4656	CE1	PHE	42	62.838	19.917	65.210	1.00	29.54
ATOM	4657	CE2	PHE	42	64.891	18.692	64.919	1.00	30.12
ATOM	4658	CZ	PHE	42	63.998	19.378	65.742	1.00	27.83
ATOM	4659	C	PHE	42	61.446	18.625	59.667	1.00	35.00
ATOM	4660	O	PHE	42	60.273	18.979	59.444	1.00	33.42
ATOM	4661	N	MET	43	62.352	18.439	58.702	1.00	36.19
ATOM	4662	H	MET	43	63.210	18.028	58.935	1.00	0.00
ATOM	4663	CA	MET	43	62.067	18.765	57.322	1.00	35.94
ATOM	4664	CB	MET	43	63.380	18.565	56.578	1.00	36.20
ATOM	4665	CG	MET	43	64.344	19.722	56.917	1.00	37.04
ATOM	4666	SD	MET	43	63.563	21.344	56.618	1.00	34.77

105/145

FIGURE 1 (CONT.)

ATOM	4667	CE	MET	43	63.748	21.469	54.860	1.00	40.60
ATOM	4668	C	MET	43	60.891	17.994	56.713	1.00	36.44
ATOM	4669	O	MET	43	60.256	18.568	55.843	1.00	37.44
ATOM	4670	N	SER	44	60.488	16.768	57.116	1.00	37.83
ATOM	4671	H	SER	44	61.071	16.277	57.728	1.00	0.00
ATOM	4672	CA	SER	44	59.219	16.162	56.645	1.00	38.34
ATOM	4673	CB	SER	44	59.127	14.653	56.891	1.00	37.41
ATOM	4674	OG	SER	44	59.265	14.146	58.207	1.00	35.40
ATOM	4675	HG	SER	44	58.681	14.602	58.827	1.00	0.00
ATOM	4676	C	SER	44	57.903	16.718	57.213	1.00	38.60
ATOM	4677	O	SER	44	56.810	16.177	57.029	1.00	37.90
ATOM	4678	N	LEU	45	57.931	17.820	57.949	1.00	39.42
ATOM	4679	H	LEU	45	58.802	18.163	58.235	1.00	0.00
ATOM	4680	CA	LEU	45	56.696	18.456	58.405	1.00	40.35
ATOM	4681	CB	LEU	45	57.044	19.103	59.765	1.00	38.21
ATOM	4682	CG	LEU	45	57.237	18.335	61.092	1.00	33.06
ATOM	4683	CD1	LEU	45	58.179	19.066	62.019	1.00	31.72
ATOM	4684	CD2	LEU	45	55.934	18.313	61.850	1.00	30.96
ATOM	4685	C	LEU	45	56.166	19.484	57.366	1.00	42.87
ATOM	4686	O	LEU	45	56.802	19.669	56.318	1.00	43.28
ATOM	4687	N	PRO	46	55.098	20.292	57.517	1.00	44.08
ATOM	4688	CD	PRO	46	53.855	19.898	58.172	1.00	45.04
ATOM	4689	CA	PRO	46	54.927	21.541	56.732	1.00	43.45
ATOM	4690	CB	PRO	46	53.444	21.797	56.823	1.00	45.31
ATOM	4691	CG	PRO	46	52.844	20.427	57.153	1.00	46.26
ATOM	4692	C	PRO	46	55.792	22.728	57.199	1.00	43.68
ATOM	4693	O	PRO	46	55.362	23.885	57.285	1.00	43.00
ATOM	4694	N	ALA	47	57.061	22.398	57.522	1.00	42.63
ATOM	4695	H	ALA	47	57.329	21.500	57.252	1.00	0.00
ATOM	4696	CA	ALA	47	58.099	23.288	58.077	1.00	41.49
ATOM	4697	CB	ALA	47	58.938	22.537	59.178	1.00	38.87
ATOM	4698	C	ALA	47	59.052	23.785	56.985	1.00	39.96
ATOM	4699	O	ALA	47	59.359	24.966	56.867	1.00	37.48
ATOM	4700	N	ALA	48	59.526	22.835	56.169	1.00	42.03
ATOM	4701	H	ALA	48	59.291	21.912	56.393	1.00	0.00
ATOM	4702	CA	ALA	48	60.314	23.056	54.930	1.00	42.00
ATOM	4703	CB	ALA	48	60.096	21.883	53.961	1.00	41.89
ATOM	4704	C	ALA	48	60.018	24.332	54.125	1.00	40.63
ATOM	4705	O	ALA	48	58.877	24.820	54.128	1.00	39.97
ATOM	4706	N	GLN	49	60.969	24.918	53.397	1.00	38.82
ATOM	4707	H	GLN	49	61.847	24.490	53.377	1.00	0.00
ATOM	4708	CA	GLN	49	60.741	26.195	52.694	1.00	39.31
ATOM	4709	CB	GLN	49	59.652	25.955	51.580	1.00	43.04
ATOM	4710	CG	GLN	49	58.662	27.003	51.064	1.00	46.76
ATOM	4711	CD	GLN	49	57.230	26.821	51.578	1.00	49.15

106/145

FIGURE 1 (CONT.)

ATOM	4712	OE1	GLN	49	56.257	27.247	50.971	1.00	50.46
ATOM	4713	NE2	GLN	49	56.877	26.201	52.673	1.00	50.49
ATOM	4714	HE21	GLN	49	57.513	25.768	53.264	1.00	0.00
ATOM	4715	HE22	GLN	49	55.910	26.242	52.789	1.00	0.00
ATOM	4716	C	GLN	49	60.385	27.381	53.600	1.00	37.90
ATOM	4717	O	GLN	49	60.813	28.491	53.303	1.00	36.12
ATOM	4718	N	ALA	50	59.652	27.283	54.715	1.00	39.42
ATOM	4719	H	ALA	50	59.242	26.437	54.981	1.00	0.00
ATOM	4720	CA	ALA	50	59.455	28.415	55.625	1.00	39.87
ATOM	4721	CB	ALA	50	58.321	28.188	56.622	1.00	43.11
ATOM	4722	C	ALA	50	60.713	28.701	56.442	1.00	38.16
ATOM	4723	O	ALA	50	61.117	28.175	57.465	1.00	35.76
ATOM	4724	N	ASN	51	61.367	29.569	55.701	1.00	39.25
ATOM	4725	H	ASN	51	60.965	29.761	54.825	1.00	0.00
ATOM	4726	CA	ASN	51	62.639	30.147	55.959	1.00	35.30
ATOM	4727	CB	ASN	51	62.416	31.139	56.990	1.00	37.03
ATOM	4728	CG	ASN	51	63.428	32.174	56.681	1.00	40.09
ATOM	4729	OD1	ASN	51	64.610	32.006	56.925	1.00	42.52
ATOM	4730	ND2	ASN	51	63.077	33.246	56.040	1.00	44.40
ATOM	4731	HD21	ASN	51	63.831	33.847	55.881	1.00	0.00
ATOM	4732	HD22	ASN	51	62.155	33.379	55.763	1.00	0.00
ATOM	4733	C	ASN	51	63.772	29.209	56.308	1.00	35.77
ATOM	4734	O	ASN	51	63.649	28.061	56.727	1.00	33.32
ATOM	4735	N	PRO	52	64.953	29.684	55.976	1.00	37.71
ATOM	4736	CD	PRO	52	65.255	30.167	54.609	1.00	43.47
ATOM	4737	CA	PRO	52	66.182	29.192	56.555	1.00	38.05
ATOM	4738	CB	PRO	52	67.256	29.796	55.696	1.00	41.31
ATOM	4739	CG	PRO	52	66.676	29.631	54.303	1.00	43.68
ATOM	4740	C	PRO	52	66.446	29.379	58.010	1.00	36.65
ATOM	4741	O	PRO	52	67.588	29.238	58.494	1.00	38.33
ATOM	4742	N	LEU	53	65.336	29.657	58.704	1.00	33.10
ATOM	4743	H	LEU	53	64.614	30.123	58.249	1.00	0.00
ATOM	4744	CA	LEU	53	65.366	29.609	60.154	1.00	28.71
ATOM	4745	CB	LEU	53	64.289	30.519	60.722	1.00	24.11
ATOM	4746	CG	LEU	53	64.727	32.007	60.528	1.00	23.96
ATOM	4747	CD1	LEU	53	63.753	32.993	61.136	1.00	18.97
ATOM	4748	CD2	LEU	53	66.087	32.193	61.157	1.00	19.94
ATOM	4749	C	LEU	53	65.246	28.202	60.679	1.00	28.10
ATOM	4750	O	LEU	53	65.829	27.975	61.723	1.00	29.34
ATOM	4751	N	VAL	54	64.697	27.174	60.016	1.00	28.55
ATOM	4752	H	VAL	54	64.172	27.372	59.208	1.00	0.00
ATOM	4753	CA	VAL	54	64.735	25.797	60.549	1.00	29.15
ATOM	4754	CB	VAL	54	63.950	24.806	59.660	1.00	27.63
ATOM	4755	CG1	VAL	54	64.220	23.283	59.776	1.00	24.44
ATOM	4756	CG2	VAL	54	62.567	25.015	60.236	1.00	27.84

107/145

FIGURE 1 (CONT.)

ATOM	4757	C	VAL	54	66.073	25.141	60.827	1.00	29.87
ATOM	4758	O	VAL	54	66.279	24.627	61.933	1.00	33.39
ATOM	4759	N	GLN	55	67.033	25.101	59.922	1.00	29.85
ATOM	4760	H	GLN	55	66.856	25.434	59.021	1.00	0.00
ATOM	4761	CA	GLN	55	68.304	24.482	60.291	1.00	29.88
ATOM	4762	CB	GLN	55	69.043	24.300	59.000	1.00	32.95
ATOM	4763	CG	GLN	55	70.414	23.622	59.011	1.00	35.84
ATOM	4764	CD	GLN	55	70.436	22.287	59.693	1.00	36.37
ATOM	4765	OE1	GLN	55	71.135	22.093	60.666	1.00	39.75
ATOM	4766	NE2	GLN	55	69.698	21.299	59.277	1.00	34.96
ATOM	4767	HE21	GLN	55	69.126	21.380	58.498	1.00	0.00
ATOM	4768	HE22	GLN	55	69.827	20.512	59.838	1.00	0.00
ATOM	4769	C	GLN	55	69.066	25.309	61.346	1.00	28.98
ATOM	4770	O	GLN	55	69.689	24.740	62.236	1.00	30.91
ATOM	4771	N	ARG	56	69.003	26.647	61.338	1.00	27.89
ATOM	4772	H	ARG	56	68.622	27.089	60.552	1.00	0.00
ATOM	4773	CA	ARG	56	69.486	27.499	62.441	1.00	26.72
ATOM	4774	CB	ARG	56	69.007	28.936	62.282	1.00	26.41
ATOM	4775	CG	ARG	56	69.659	29.756	61.192	1.00	24.38
ATOM	4776	CD	ARG	56	70.952	30.345	61.758	1.00	29.01
ATOM	4777	NE	ARG	56	72.034	29.380	61.906	1.00	29.18
ATOM	4778	HE	ARG	56	72.154	28.707	61.203	1.00	0.00
ATOM	4779	CZ	ARG	56	72.884	29.362	62.926	1.00	27.05
ATOM	4780	NH1	ARG	56	73.800	28.411	62.935	1.00	29.23
ATOM	4781	HH11	ARG	56	74.454	28.362	63.690	1.00	0.00
ATOM	4782	HH12	ARG	56	73.838	27.739	62.196	1.00	0.00
ATOM	4783	NH2	ARG	56	72.860	30.249	63.905	1.00	25.94
ATOM	4784	HH21	ARG	56	72.172	30.974	63.902	1.00	0.00
ATOM	4785	HH22	ARG	56	73.517	30.189	64.656	1.00	0.00
ATOM	4786	C	ARG	56	68.973	27.022	63.807	1.00	26.27
ATOM	4787	O	ARG	56	69.749	26.616	64.665	1.00	24.82
ATOM	4788	N	VAL	57	67.640	26.938	63.952	1.00	26.24
ATOM	4789	H	VAL	57	67.091	27.206	63.184	1.00	0.00
ATOM	4790	CA	VAL	57	66.972	26.481	65.160	1.00	25.79
ATOM	4791	CB	VAL	57	65.466	26.552	64.962	1.00	28.37
ATOM	4792	CG1	VAL	57	64.787	26.100	66.254	1.00	32.19
ATOM	4793	CG2	VAL	57	65.003	27.996	64.675	1.00	27.17
ATOM	4794	C	VAL	57	67.360	25.076	65.581	1.00	25.61
ATOM	4795	O	VAL	57	67.585	24.871	66.768	1.00	25.38
ATOM	4796	N	ILE	58	67.479	24.096	64.678	1.00	27.36
ATOM	4797	H	ILE	58	67.162	24.279	63.769	1.00	0.00
ATOM	4798	CA	ILE	58	68.045	22.768	65.012	1.00	27.73
ATOM	4799	CB	ILE	58	68.134	21.810	63.770	1.00	29.70
ATOM	4800	CG2	ILE	58	68.673	20.428	64.164	1.00	29.51
ATOM	4801	CG1	ILE	58	66.753	21.608	63.187	1.00	30.90

108/145

FIGURE 1 (CONT.)

ATOM	4802	CD1	ILE	58	66.655	20.797	61.890	1.00	29.63
ATOM	4803	C	ILE	58	69.465	22.918	65.574	1.00	27.65
ATOM	4804	O	ILE	58	69.786	22.424	66.658	1.00	27.43
ATOM	4805	N	ASP	59	70.323	23.692	64.915	1.00	29.50
ATOM	4806	H	ASP	59	70.048	24.070	64.051	1.00	0.00
ATOM	4807	CA	ASP	59	71.690	23.908	65.399	1.00	30.63
ATOM	4808	CB	ASP	59	72.453	24.726	64.337	1.00	30.52
ATOM	4809	CG	ASP	59	72.600	23.878	63.070	1.00	32.62
ATOM	4810	OD1	ASP	59	72.680	22.653	63.173	1.00	34.14
ATOM	4811	OD2	ASP	59	72.628	24.416	61.968	1.00	33.24
ATOM	4812	C	ASP	59	71.800	24.556	66.773	1.00	31.09
ATOM	4813	O	ASP	59	72.611	24.136	67.612	1.00	31.17
ATOM	4814	N	ILE	60	70.909	25.520	67.064	1.00	29.67
ATOM	4815	H	ILE	60	70.326	25.835	66.342	1.00	0.00
ATOM	4816	CA	ILE	60	70.895	26.107	68.397	1.00	27.03
ATOM	4817	CB	ILE	60	70.127	27.412	68.330	1.00	23.72
ATOM	4818	CG2	ILE	60	70.031	28.087	69.695	1.00	24.77
ATOM	4819	CG1	ILE	60	70.870	28.320	67.401	1.00	17.79
ATOM	4820	CD1	ILE	60	70.019	29.539	67.147	1.00	16.29
ATOM	4821	C	ILE	60	70.302	25.155	69.449	1.00	27.91
ATOM	4822	O	ILE	60	70.821	25.104	70.576	1.00	29.66
ATOM	4823	N	PHE	61	69.264	24.362	69.086	1.00	25.45
ATOM	4824	H	PHE	61	68.884	24.483	68.190	1.00	0.00
ATOM	4825	CA	PHE	61	68.691	23.356	69.986	1.00	22.23
ATOM	4826	CB	PHE	61	67.411	22.746	69.423	1.00	19.37
ATOM	4827	CG	PHE	61	66.106	23.532	69.583	1.00	17.84
ATOM	4828	CD1	PHE	61	64.901	22.822	69.552	1.00	18.49
ATOM	4829	CD2	PHE	61	66.076	24.930	69.737	1.00	20.62
ATOM	4830	CE1	PHE	61	63.677	23.477	69.662	1.00	17.14
ATOM	4831	CE2	PHE	61	64.853	25.598	69.855	1.00	20.70
ATOM	4832	CZ	PHE	61	63.656	24.866	69.811	1.00	21.06
ATOM	4833	C	PHE	61	69.676	22.234	70.223	1.00	22.94
ATOM	4834	O	PHE	61	69.684	21.569	71.241	1.00	23.72
ATOM	4835	N	ASP	62	70.574	22.052	69.285	1.00	25.47
ATOM	4836	H	ASP	62	70.508	22.617	68.488	1.00	0.00
ATOM	4837	CA	ASP	62	71.628	21.052	69.310	1.00	27.41
ATOM	4838	CB	ASP	62	72.160	20.886	67.898	1.00	27.53
ATOM	4839	CG	ASP	62	72.771	19.532	67.656	1.00	28.86
ATOM	4840	OD1	ASP	62	73.945	19.322	67.915	1.00	28.91
ATOM	4841	OD2	ASP	62	72.036	18.665	67.211	1.00	31.95
ATOM	4842	C	ASP	62	72.786	21.374	70.236	1.00	28.90
ATOM	4843	O	ASP	62	73.952	21.277	69.835	1.00	30.31
ATOM	4844	N	THR	63	72.565	21.674	71.513	1.00	29.59
ATOM	4845	H	THR	63	71.649	21.615	71.856	1.00	0.00
ATOM	4846	CA	THR	63	73.693	22.108	72.357	1.00	31.16

109/145

FIGURE 1 (CONT.)

ATOM	4847	CB	THR	63	73.268	22.306	73.802	1.00	27.05
ATOM	4848	OG1	THR	63	72.814	21.073	74.311	1.00	30.92
ATOM	4849	HG1	THR	63	72.455	21.222	75.196	1.00	0.00
ATOM	4850	CG2	THR	63	72.188	23.329	73.891	1.00	25.87
ATOM	4851	C	THR	63	74.942	21.234	72.386	1.00	32.49
ATOM	4852	O	THR	63	76.047	21.741	72.206	1.00	32.96
ATOM	4853	N	ASP	64	74.836	19.906	72.459	1.00	36.46
ATOM	4854	H	ASP	64	73.938	19.531	72.560	1.00	0.00
ATOM	4855	CA	ASP	64	76.055	19.065	72.483	1.00	38.79
ATOM	4856	CB	ASP	64	75.769	17.732	73.135	1.00	41.46
ATOM	4857	CG	ASP	64	75.061	16.776	72.202	1.00	42.82
ATOM	4858	OD1	ASP	64	74.103	17.209	71.590	1.00	40.12
ATOM	4859	OD2	ASP	64	75.502	15.632	72.077	1.00	48.32
ATOM	4860	C	ASP	64	76.742	18.753	71.155	1.00	37.76
ATOM	4861	O	ASP	64	77.508	17.789	71.001	1.00	38.18
ATOM	4862	N	GLY	65	76.347	19.492	70.131	1.00	37.16
ATOM	4863	H	GLY	65	75.662	20.185	70.252	1.00	0.00
ATOM	4864	CA	GLY	65	77.007	19.332	68.846	1.00	36.17
ATOM	4865	C	GLY	65	76.661	18.095	68.052	1.00	33.75
ATOM	4866	O	GLY	65	77.073	18.089	66.912	1.00	35.07
ATOM	4867	N	ASN	66	75.871	17.075	68.424	1.00	35.08
ATOM	4868	H	ASN	66	75.559	17.024	69.349	1.00	0.00
ATOM	4869	CA	ASN	66	75.719	15.929	67.494	1.00	33.84
ATOM	4870	CB	ASN	66	75.561	14.608	68.335	1.00	36.20
ATOM	4871	CG	ASN	66	74.281	14.223	69.056	1.00	37.54
ATOM	4872	OD1	ASN	66	73.841	14.864	69.989	1.00	40.92
ATOM	4873	ND2	ASN	66	73.595	13.148	68.747	1.00	38.66
ATOM	4874	HD21	ASN	66	73.879	12.590	68.005	1.00	0.00
ATOM	4875	HD22	ASN	66	72.830	12.994	69.334	1.00	0.00
ATOM	4876	C	ASN	66	74.699	15.913	66.349	1.00	29.58
ATOM	4877	O	ASN	66	74.259	14.863	65.859	1.00	30.26
ATOM	4878	N	GLY	67	74.323	17.082	65.864	1.00	24.27
ATOM	4879	H	GLY	67	74.772	17.877	66.216	1.00	0.00
ATOM	4880	CA	GLY	67	73.398	17.170	64.742	1.00	22.85
ATOM	4881	C	GLY	67	71.898	16.881	64.907	1.00	23.84
ATOM	4882	O	GLY	67	71.041	17.499	64.260	1.00	23.40
ATOM	4883	N	GLY	68	71.499	15.921	65.730	1.00	25.27
ATOM	4884	H	GLY	68	72.184	15.345	66.126	1.00	0.00
ATOM	4885	CA	GLY	68	70.076	15.679	65.960	1.00	24.34
ATOM	4886	C	GLY	68	69.609	16.327	67.254	1.00	26.00
ATOM	4887	O	GLY	68	70.302	16.371	68.263	1.00	24.97
ATOM	4888	N	VAL	69	68.426	16.864	67.356	1.00	27.40
ATOM	4889	H	VAL	69	67.863	16.916	66.552	1.00	0.00
ATOM	4890	CA	VAL	69	67.996	17.404	68.640	1.00	28.53
ATOM	4891	CB	VAL	69	66.939	18.488	68.317	1.00	28.35

110/145

FIGURE 1 (CONT.)

ATOM	4892	CG1	VAL	69	66.562	19.169	69.597	1.00	30.00
ATOM	4893	CG2	VAL	69	67.485	19.554	67.365	1.00	25.07
ATOM	4894	C	VAL	69	67.485	16.310	69.609	1.00	29.91
ATOM	4895	O	VAL	69	66.398	15.784	69.419	1.00	30.66
ATOM	4896	N	ASP	70	68.206	15.810	70.627	1.00	31.42
ATOM	4897	H	ASP	70	69.149	16.073	70.660	1.00	0.00
ATOM	4898	CA	ASP	70	67.650	14.846	71.607	1.00	30.14
ATOM	4899	CB	ASP	70	68.795	14.348	72.562	1.00	32.22
ATOM	4900	CG	ASP	70	69.533	15.249	73.573	1.00	32.20
ATOM	4901	OD1	ASP	70	70.745	15.127	73.730	1.00	36.10
ATOM	4902	OD2	ASP	70	68.921	16.048	74.261	1.00	33.14
ATOM	4903	C	ASP	70	66.449	15.301	72.474	1.00	30.31
ATOM	4904	O	ASP	70	66.166	16.495	72.491	1.00	33.09
ATOM	4905	N	PHE	71	65.688	14.512	73.259	1.00	27.47
ATOM	4906	H	PHE	71	65.814	13.545	73.187	1.00	0.00
ATOM	4907	CA	PHE	71	64.583	15.045	74.055	1.00	23.77
ATOM	4908	CB	PHE	71	63.841	13.896	74.725	1.00	22.90
ATOM	4909	CG	PHE	71	62.600	14.336	75.496	1.00	22.35
ATOM	4910	CD1	PHE	71	62.548	14.144	76.884	1.00	22.82
ATOM	4911	CD2	PHE	71	61.548	14.982	74.839	1.00	21.06
ATOM	4912	CE1	PHE	71	61.462	14.598	77.629	1.00	19.30
ATOM	4913	CE2	PHE	71	60.462	15.433	75.583	1.00	21.43
ATOM	4914	CZ	PHE	71	60.419	15.244	76.972	1.00	22.04
ATOM	4915	C	PHE	71	64.985	16.078	75.111	1.00	25.41
ATOM	4916	O	PHE	71	64.254	17.059	75.269	1.00	26.02
ATOM	4917	N	LYS	72	66.102	15.989	75.858	1.00	25.13
ATOM	4918	H	LYS	72	66.612	15.154	75.841	1.00	0.00
ATOM	4919	CA	LYS	72	66.501	17.096	76.760	1.00	24.45
ATOM	4920	CB	LYS	72	67.846	16.833	77.420	1.00	24.51
ATOM	4921	CG	LYS	72	68.596	18.006	78.023	1.00	21.28
ATOM	4922	CD	LYS	72	69.876	17.542	78.703	1.00	25.45
ATOM	4923	CE	LYS	72	70.655	18.784	79.080	1.00	27.81
ATOM	4924	NZ	LYS	72	71.497	18.588	80.248	1.00	28.70
ATOM	4925	HZ1	LYS	72	72.017	19.466	80.448	1.00	0.00
ATOM	4926	HZ2	LYS	72	72.174	17.821	80.060	1.00	0.00
ATOM	4927	HZ3	LYS	72	70.914	18.340	81.073	1.00	0.00
ATOM	4928	C	LYS	72	66.624	18.432	76.046	1.00	25.42
ATOM	4929	O	LYS	72	66.121	19.470	76.490	1.00	28.71
ATOM	4930	N	GLU	73	67.269	18.380	74.890	1.00	23.15
ATOM	4931	H	GLU	73	67.559	17.513	74.569	1.00	0.00
ATOM	4932	CA	GLU	73	67.446	19.553	74.065	1.00	21.70
ATOM	4933	CB	GLU	73	68.391	19.308	72.971	1.00	25.79
ATOM	4934	CG	GLU	73	69.833	18.977	73.327	1.00	26.84
ATOM	4935	CD	GLU	73	70.626	18.572	72.099	1.00	27.35
ATOM	4936	OE1	GLU	73	70.021	18.046	71.161	1.00	27.09

111/145

FIGURE 1 (CONT.)

ATOM	4937	OE2	GLU	73	71.846	18.787	72.089	1.00	29.72
ATOM	4938	C	GLU	73	66.160	19.989	73.406	1.00	19.96
ATOM	4939	O	GLU	73	65.998	21.171	73.133	1.00	23.87
ATOM	4940	N	PHE	74	65.218	19.110	73.133	1.00	15.49
ATOM	4941	H	PHE	74	65.428	18.158	73.190	1.00	0.00
ATOM	4942	CA	PHE	74	63.931	19.531	72.645	1.00	16.50
ATOM	4943	CB	PHE	74	63.149	18.268	72.256	1.00	19.77
ATOM	4944	CG	PHE	74	61.725	18.509	71.737	1.00	22.83
ATOM	4945	CD1	PHE	74	61.519	18.992	70.432	1.00	23.10
ATOM	4946	CD2	PHE	74	60.626	18.280	72.584	1.00	21.59
ATOM	4947	CE1	PHE	74	60.212	19.250	69.988	1.00	24.60
ATOM	4948	CE2	PHE	74	59.337	18.541	72.133	1.00	21.78
ATOM	4949	CZ	PHE	74	59.122	19.027	70.838	1.00	24.23
ATOM	4950	C	PHE	74	63.212	20.361	73.716	1.00	17.83
ATOM	4951	O	PHE	74	62.683	21.433	73.406	1.00	16.95
ATOM	4952	N	ILE	75	63.212	19.892	74.990	1.00	19.54
ATOM	4953	H	ILE	75	63.585	18.995	75.112	1.00	0.00
ATOM	4954	CA	ILE	75	62.664	20.597	76.172	1.00	18.64
ATOM	4955	CB	ILE	75	62.690	19.628	77.407	1.00	19.68
ATOM	4956	CG2	ILE	75	62.228	20.312	78.718	1.00	19.97
ATOM	4957	CG1	ILE	75	61.751	18.486	77.132	1.00	16.06
ATOM	4958	CD1	ILE	75	60.285	18.853	76.886	1.00	13.75
ATOM	4959	C	ILE	75	63.354	21.916	76.561	1.00	18.00
ATOM	4960	O	ILE	75	62.736	22.965	76.749	1.00	16.91
ATOM	4961	N	GLU	76	64.662	21.855	76.764	1.00	20.17
ATOM	4962	H	GLU	76	65.079	20.976	76.786	1.00	0.00
ATOM	4963	CA	GLU	76	65.473	23.046	77.028	1.00	21.98
ATOM	4964	CB	GLU	76	66.930	22.608	77.076	1.00	23.44
ATOM	4965	CG	GLU	76	67.491	22.815	78.450	1.00	27.67
ATOM	4966	CD	GLU	76	68.336	21.682	78.998	1.00	29.76
ATOM	4967	OE1	GLU	76	69.556	21.760	78.940	1.00	30.95
ATOM	4968	OE2	GLU	76	67.773	20.731	79.529	1.00	33.60
ATOM	4969	C	GLU	76	65.253	24.130	75.958	1.00	22.04
ATOM	4970	O	GLU	76	64.851	25.255	76.278	1.00	22.30
ATOM	4971	N	GLY	77	65.403	23.719	74.671	1.00	20.48
ATOM	4972	H	GLY	77	65.743	22.811	74.545	1.00	0.00
ATOM	4973	CA	GLY	77	65.169	24.550	73.494	1.00	16.85
ATOM	4974	C	GLY	77	63.773	25.164	73.406	1.00	17.32
ATOM	4975	O	GLY	77	63.625	26.356	73.179	1.00	17.28
ATOM	4976	N	VAL	78	62.677	24.425	73.544	1.00	19.21
ATOM	4977	H	VAL	78	62.787	23.453	73.650	1.00	0.00
ATOM	4978	CA	VAL	78	61.347	25.048	73.495	1.00	20.86
ATOM	4979	CB	VAL	78	60.237	23.985	73.330	1.00	20.81
ATOM	4980	CG1	VAL	78	58.905	24.671	73.036	1.00	18.46
ATOM	4981	CG2	VAL	78	60.589	23.043	72.204	1.00	22.50

112/145

**FIGURE 1 (CONT.)**

ATOM	4982	C	VAL	78	61.034	25.884	74.748	1.00	23.71
ATOM	4983	O	VAL	78	60.215	26.801	74.621	1.00	25.45
ATOM	4984	N	MET	79	61.628	25.597	75.950	1.00	24.32
ATOM	4985	H	MET	79	62.192	24.793	75.985	1.00	0.00
ATOM	4986	CA	MET	79	61.510	26.409	77.174	1.00	24.58
ATOM	4987	CB	MET	79	62.340	25.751	78.300	1.00	29.49
ATOM	4988	CG	MET	79	62.811	26.609	79.487	1.00	36.70
ATOM	4989	SD	MET	79	64.621	26.923	79.690	1.00	48.09
ATOM	4990	CE	MET	79	64.794	27.963	81.145	1.00	41.05
ATOM	4991	C	MET	79	61.949	27.867	77.009	1.00	22.64
ATOM	4992	O	MET	79	61.413	28.721	77.705	1.00	20.32
ATOM	4993	N	GLN	80	62.952	28.226	76.180	1.00	23.59
ATOM	4994	H	GLN	80	63.527	27.497	75.851	1.00	0.00
ATOM	4995	CA	GLN	80	63.276	29.634	75.906	1.00	24.86
ATOM	4996	CB	GLN	80	64.369	29.815	74.865	1.00	24.27
ATOM	4997	CG	GLN	80	65.557	28.925	74.812	1.00	23.03
ATOM	4998	CD	GLN	80	66.095	28.678	76.189	1.00	26.50
ATOM	4999	OE1	GLN	80	65.893	27.629	76.783	1.00	27.80
ATOM	5000	NE2	GLN	80	66.802	29.603	76.801	1.00	28.20
ATOM	5001	HE21	GLN	80	67.022	30.435	76.329	1.00	0.00
ATOM	5002	HE22	GLN	80	67.134	29.324	77.676	1.00	0.00
ATOM	5003	C	GLN	80	62.084	30.432	75.342	1.00	27.04
ATOM	5004	O	GLN	80	61.949	31.635	75.516	1.00	28.64
ATOM	5005	N	PHE	81	61.162	29.742	74.688	1.00	29.96
ATOM	5006	H	PHE	81	61.265	28.768	74.648	1.00	0.00
ATOM	5007	CA	PHE	81	59.979	30.303	74.064	1.00	30.84
ATOM	5008	CB	PHE	81	59.758	29.641	72.711	1.00	32.21
ATOM	5009	CG	PHE	81	60.998	29.760	71.850	1.00	35.32
ATOM	5010	CD1	PHE	81	61.971	28.759	71.888	1.00	34.31
ATOM	5011	CD2	PHE	81	61.143	30.874	71.018	1.00	36.97
ATOM	5012	CE1	PHE	81	63.089	28.871	71.082	1.00	32.83
ATOM	5013	CE2	PHE	81	62.269	30.977	70.217	1.00	34.22
ATOM	5014	CZ	PHE	81	63.226	29.977	70.254	1.00	34.39
ATOM	5015	C	PHE	81	58.743	30.112	74.897	1.00	30.57
ATOM	5016	O	PHE	81	57.886	29.352	74.504	1.00	33.66
ATOM	5017	N	VAL	82	58.537	30.740	76.042	1.00	32.34
ATOM	5018	H	VAL	82	59.243	31.346	76.337	1.00	0.00
ATOM	5019	CA	VAL	82	57.307	30.550	76.793	1.00	31.03
ATOM	5020	CB	VAL	82	57.423	29.149	77.500	1.00	31.67
ATOM	5021	CG1	VAL	82	58.097	29.216	78.845	1.00	31.98
ATOM	5022	CG2	VAL	82	56.019	28.571	77.610	1.00	34.97
ATOM	5023	C	VAL	82	57.102	31.726	77.740	1.00	31.27
ATOM	5024	O	VAL	82	55.963	32.098	78.089	1.00	32.61
ATOM	5025	CB	LYS	84	56.980	30.500	81.933	1.00	21.43
ATOM	5026	CG	LYS	84	55.808	30.277	82.848	1.00	21.83

113/145

FIGURE 1 (CONT.)

ATOM	5027	CD	LYS	84	55.648	28.776	83.111	1.00	27.02
ATOM	5028	CE	LYS	84	55.174	27.866	81.945	1.00	32.18
ATOM	5029	NZ	LYS	84	56.055	27.700	80.787	1.00	32.47
ATOM	5030	HZ1	LYS	84	56.953	27.274	81.095	1.00	0.00
ATOM	5031	HZ2	LYS	84	56.240	28.630	80.363	1.00	0.00
ATOM	5032	HZ3	LYS	84	55.604	27.084	80.084	1.00	0.00
ATOM	5033	C	LYS	84	58.631	32.084	81.041	1.00	24.32
ATOM	5034	O	LYS	84	59.415	31.883	81.960	1.00	27.07
ATOM	5035	HT1	LYS	84	55.117	32.236	81.158	1.00	0.00
ATOM	5036	HT2	LYS	84	55.865	31.551	79.810	1.00	0.00
ATOM	5037	N	LYS	84	55.999	32.231	80.593	1.00	24.15
ATOM	5038	HT3	LYS	84	56.079	33.155	80.120	1.00	0.00
ATOM	5039	CA	LYS	84	57.147	31.913	81.449	1.00	23.63
ATOM	5040	N	GLY	85	59.176	32.422	79.854	1.00	22.00
ATOM	5041	H	GLY	85	58.610	32.700	79.110	1.00	0.00
ATOM	5042	CA	GLY	85	60.616	32.702	79.704	1.00	22.40
ATOM	5043	C	GLY	85	60.918	34.213	79.650	1.00	23.71
ATOM	5044	O	GLY	85	59.958	34.897	79.289	1.00	25.16
ATOM	5045	N	ASP	86	62.051	34.906	79.944	1.00	26.27
ATOM	5046	H	ASP	86	62.857	34.419	80.208	1.00	0.00
ATOM	5047	CA	ASP	86	62.070	36.392	79.799	1.00	27.84
ATOM	5048	CB	ASP	86	62.359	37.112	81.179	1.00	29.81
ATOM	5049	CG	ASP	86	62.103	38.651	81.276	1.00	33.67
ATOM	5050	OD1	ASP	86	63.002	39.403	81.679	1.00	34.79
ATOM	5051	OD2	ASP	86	61.011	39.131	80.938	1.00	35.92
ATOM	5052	C	ASP	86	63.023	37.000	78.757	1.00	26.96
ATOM	5053	O	ASP	86	63.932	36.353	78.259	1.00	28.38
ATOM	5054	N	LYS	87	62.812	38.270	78.398	1.00	26.64
ATOM	5055	H	LYS	87	62.032	38.684	78.814	1.00	0.00
ATOM	5056	CA	LYS	87	63.515	39.038	77.389	1.00	26.57
ATOM	5057	CB	LYS	87	63.348	40.521	77.837	1.00	28.92
ATOM	5058	CG	LYS	87	64.160	41.790	77.479	1.00	29.28
ATOM	5059	CD	LYS	87	65.313	41.972	78.516	1.00	35.56
ATOM	5060	CE	LYS	87	64.873	42.020	80.040	1.00	38.72
ATOM	5061	NZ	LYS	87	65.921	41.646	81.009	1.00	34.40
ATOM	5062	HZ1	LYS	87	66.703	42.330	80.971	1.00	0.00
ATOM	5063	HZ2	LYS	87	66.287	40.698	80.783	1.00	0.00
ATOM	5064	HZ3	LYS	87	65.530	41.630	81.971	1.00	0.00
ATOM	5065	C	LYS	87	64.932	38.576	77.181	1.00	27.53
ATOM	5066	O	LYS	87	65.257	38.130	76.091	1.00	31.48
ATOM	5067	N	GLU	88	65.727	38.403	78.223	1.00	27.03
ATOM	5068	H	GLU	88	65.370	38.570	79.114	1.00	0.00
ATOM	5069	CA	GLU	88	67.122	37.986	78.035	1.00	27.90
ATOM	5070	CB	GLU	88	67.854	38.078	79.344	1.00	29.77
ATOM	5071	CG	GLU	88	69.367	37.905	79.198	1.00	28.70

114/145

FIGURE 1 (CONT.)

ATOM	5072	CD	GLU	88	70.077	37.855	80.525	1.00	26.54
ATOM	5073	OE1	GLU	88	69.643	38.470	81.496	1.00	23.30
ATOM	5074	OE2	GLU	88	71.067	37.150	80.563	1.00	27.08
ATOM	5075	C	GLU	88	67.428	36.612	77.456	1.00	26.23
ATOM	5076	O	GLU	88	68.353	36.488	76.669	1.00	26.81
ATOM	5077	N	GLN	89	66.750	35.537	77.823	1.00	27.26
ATOM	5078	H	GLN	89	66.034	35.646	78.485	1.00	0.00
ATOM	5079	CA	GLN	89	67.013	34.242	77.178	1.00	30.08
ATOM	5080	CB	GLN	89	66.408	33.032	77.972	1.00	30.56
ATOM	5081	CG	GLN	89	64.892	32.963	78.354	1.00	31.83
ATOM	5082	CD	GLN	89	64.524	31.740	79.202	1.00	26.96
ATOM	5083	OE1	GLN	89	63.788	31.804	80.172	1.00	25.64
ATOM	5084	NE2	GLN	89	64.990	30.550	78.922	1.00	24.46
ATOM	5085	HE21	GLN	89	64.716	29.817	79.491	1.00	0.00
ATOM	5086	HE22	GLN	89	65.566	30.460	78.142	1.00	0.00
ATOM	5087	C	GLN	89	66.423	34.265	75.763	1.00	29.96
ATOM	5088	O	GLN	89	67.042	33.791	74.816	1.00	29.12
ATOM	5089	N	LYS	90	65.265	34.910	75.581	1.00	30.48
ATOM	5090	H	LYS	90	64.799	35.277	76.364	1.00	0.00
ATOM	5091	CA	LYS	90	64.694	35.126	74.255	1.00	29.75
ATOM	5092	CB	LYS	90	63.320	35.762	74.376	1.00	28.54
ATOM	5093	CG	LYS	90	62.330	34.820	75.060	1.00	27.21
ATOM	5094	CD	LYS	90	60.987	35.544	75.221	1.00	28.59
ATOM	5095	CE	LYS	90	59.938	34.674	75.882	1.00	25.81
ATOM	5096	NZ	LYS	90	59.737	33.456	75.124	1.00	27.36
ATOM	5097	HZ1	LYS	90	59.436	33.727	74.168	1.00	0.00
ATOM	5098	HZ2	LYS	90	59.003	32.870	75.570	1.00	0.00
ATOM	5099	HZ3	LYS	90	60.624	32.921	75.060	1.00	0.00
ATOM	5100	C	LYS	90	65.598	36.025	73.421	1.00	28.62
ATOM	5101	O	LYS	90	65.580	35.939	72.194	1.00	29.68
ATOM	5102	N	LEU	91	66.470	36.844	74.020	1.00	28.09
ATOM	5103	H	LEU	91	66.352	37.028	74.969	1.00	0.00
ATOM	5104	CA	LEU	91	67.441	37.611	73.218	1.00	30.27
ATOM	5105	CB	LEU	91	67.594	39.011	73.790	1.00	30.59
ATOM	5106	CG	LEU	91	66.581	39.966	73.185	1.00	31.11
ATOM	5107	CD1	LEU	91	66.497	41.228	73.992	1.00	32.24
ATOM	5108	CD2	LEU	91	67.006	40.274	71.750	1.00	32.70
ATOM	5109	C	LEU	91	68.825	36.986	73.033	1.00	30.77
ATOM	5110	O	LEU	91	69.498	37.172	72.010	1.00	31.76
ATOM	5111	N	ARG	92	69.250	36.179	74.000	1.00	28.76
ATOM	5112	H	ARG	92	68.840	36.250	74.881	1.00	0.00
ATOM	5113	CA	ARG	92	70.355	35.271	73.787	1.00	27.29
ATOM	5114	CB	ARG	92	70.659	34.407	74.994	1.00	28.38
ATOM	5115	CG	ARG	92	71.140	35.124	76.222	1.00	29.93
ATOM	5116	CD	ARG	92	72.641	34.866	76.362	1.00	35.29

115/145

FIGURE 1 (CONT.)

ATOM	5117	NE	ARG	92	73.286	35.926	77.133	1.00	37.73
ATOM	5118	HE	ARG	92	73.942	36.498	76.686	1.00	0.00
ATOM	5119	CZ	ARG	92	73.045	36.119	78.430	1.00	37.81
ATOM	5120	NH1	ARG	92	73.600	37.160	79.045	1.00	36.85
ATOM	5121	HH11	ARG	92	74.196	37.786	78.540	1.00	0.00
ATOM	5122	HH12	ARG	92	73.407	37.322	80.013	1.00	0.00
ATOM	5123	NH2	ARG	92	72.293	35.267	79.131	1.00	38.94
ATOM	5124	HH21	ARG	92	72.106	35.443	80.097	1.00	0.00
ATOM	5125	HH22	ARG	92	71.878	34.476	78.682	1.00	0.00
ATOM	5126	C	ARG	92	69.935	34.308	72.676	1.00	27.47
ATOM	5127	O	ARG	92	70.797	33.868	71.916	1.00	31.19
ATOM	5128	N	PHE	93	68.658	33.920	72.481	1.00	25.84
ATOM	5129	H	PHE	93	67.987	34.190	73.141	1.00	0.00
ATOM	5130	CA	PHE	93	68.328	33.003	71.377	1.00	25.52
ATOM	5131	CB	PHE	93	66.854	32.505	71.412	1.00	26.81
ATOM	5132	CG	PHE	93	66.586	31.324	70.444	1.00	28.33
ATOM	5133	CD1	PHE	93	66.825	30.006	70.853	1.00	27.70
ATOM	5134	CD2	PHE	93	66.073	31.546	69.149	1.00	27.39
ATOM	5135	CE1	PHE	93	66.545	28.941	69.984	1.00	26.87
ATOM	5136	CE2	PHE	93	65.801	30.481	68.297	1.00	24.09
ATOM	5137	CZ	PHE	93	66.034	29.178	68.711	1.00	25.45
ATOM	5138	C	PHE	93	68.554	33.719	70.050	1.00	25.02
ATOM	5139	O	PHE	93	69.344	33.283	69.207	1.00	23.28
ATOM	5140	N	ALA	94	67.886	34.876	69.942	1.00	24.06
ATOM	5141	H	ALA	94	67.254	35.095	70.660	1.00	0.00
ATOM	5142	CA	ALA	94	67.999	35.787	68.823	1.00	21.59
ATOM	5143	CB	ALA	94	67.399	37.102	69.249	1.00	22.43
ATOM	5144	C	ALA	94	69.458	35.965	68.435	1.00	21.63
ATOM	5145	O	ALA	94	69.840	35.697	67.294	1.00	25.22
ATOM	5146	N	PHE	95	70.315	36.313	69.395	1.00	20.00
ATOM	5147	H	PHE	95	69.946	36.556	70.269	1.00	0.00
ATOM	5148	CA	PHE	95	71.770	36.403	69.185	1.00	18.95
ATOM	5149	CB	PHE	95	72.535	36.539	70.518	1.00	15.37
ATOM	5150	CG	PHE	95	73.996	36.878	70.267	1.00	17.36
ATOM	5151	CD1	PHE	95	74.331	38.166	69.875	1.00	17.17
ATOM	5152	CD2	PHE	95	74.989	35.906	70.379	1.00	17.58
ATOM	5153	CE1	PHE	95	75.639	38.480	69.592	1.00	17.94
ATOM	5154	CE2	PHE	95	76.307	36.232	70.092	1.00	16.57
ATOM	5155	CZ	PHE	95	76.639	37.518	69.696	1.00	19.91
ATOM	5156	C	PHE	95	72.357	35.192	68.473	1.00	17.92
ATOM	5157	O	PHE	95	73.104	35.281	67.509	1.00	17.70
ATOM	5158	N	ARG	96	71.939	34.031	68.944	1.00	21.05
ATOM	5159	H	ARG	96	71.293	34.038	69.682	1.00	0.00
ATOM	5160	CA	ARG	96	72.400	32.767	68.431	1.00	21.58
ATOM	5161	CB	ARG	96	71.943	31.717	69.408	1.00	23.33

116/145

FIGURE 1 (CONT.)

ATOM	5162	CG	ARG	96	72.804	31.854	70.655	1.00	28.61
ATOM	5163	CD	ARG	96	72.487	30.914	71.809	1.00	37.68
ATOM	5164	NE	ARG	96	72.542	29.455	71.555	1.00	47.07
ATOM	5165	HE	ARG	96	71.771	28.940	71.864	1.00	0.00
ATOM	5166	CZ	ARG	96	73.530	28.737	70.933	1.00	49.16
ATOM	5167	NH1	ARG	96	73.378	27.389	70.893	1.00	50.86
ATOM	5168	HH11	ARG	96	72.564	26.966	71.295	1.00	0.00
ATOM	5169	HH12	ARG	96	74.074	26.821	70.451	1.00	0.00
ATOM	5170	NH2	ARG	96	74.606	29.290	70.313	1.00	45.62
ATOM	5171	HH21	ARG	96	75.302	28.702	69.902	1.00	0.00
ATOM	5172	HH22	ARG	96	74.723	30.283	70.302	1.00	0.00
ATOM	5173	C	ARG	96	71.968	32.476	67.003	1.00	22.27
ATOM	5174	O	ARG	96	72.678	31.758	66.288	1.00	23.11
ATOM	5175	N	ILE	97	70.887	33.100	66.519	1.00	21.62
ATOM	5176	H	ILE	97	70.360	33.638	67.144	1.00	0.00
ATOM	5177	CA	ILE	97	70.479	32.941	65.129	1.00	21.50
ATOM	5178	CB	ILE	97	69.098	33.653	64.922	1.00	22.99
ATOM	5179	CG2	ILE	97	68.778	33.789	63.411	1.00	23.49
ATOM	5180	CG1	ILE	97	67.953	32.830	65.609	1.00	23.98
ATOM	5181	CD1	ILE	97	67.588	31.445	64.978	1.00	21.89
ATOM	5182	C	ILE	97	71.552	33.492	64.181	1.00	21.60
ATOM	5183	O	ILE	97	71.857	32.888	63.147	1.00	23.87
ATOM	5184	N	TYR	98	72.204	34.609	64.490	1.00	19.64
ATOM	5185	H	TYR	98	71.977	35.050	65.334	1.00	0.00
ATOM	5186	CA	TYR	98	73.222	35.154	63.592	1.00	18.71
ATOM	5187	CB	TYR	98	73.235	36.671	63.671	1.00	17.53
ATOM	5188	CG	TYR	98	71.907	37.415	63.622	1.00	15.18
ATOM	5189	CD1	TYR	98	71.378	37.780	62.398	1.00	15.27
ATOM	5190	CE1	TYR	98	70.158	38.471	62.354	1.00	18.26
ATOM	5191	CD2	TYR	98	71.217	37.734	64.802	1.00	17.20
ATOM	5192	CE2	TYR	98	69.997	38.418	64.765	1.00	17.93
ATOM	5193	CZ	TYR	98	69.471	38.790	63.529	1.00	18.96
ATOM	5194	OH	TYR	98	68.286	39.504	63.448	1.00	20.27
ATOM	5195	HH	TYR	98	68.161	39.835	62.547	1.00	0.00
ATOM	5196	C	TYR	98	74.627	34.630	63.944	1.00	21.68
ATOM	5197	O	TYR	98	75.573	34.573	63.149	1.00	20.70
ATOM	5198	N	ASP	99	74.820	34.226	65.199	1.00	23.41
ATOM	5199	H	ASP	99	74.060	34.272	65.816	1.00	0.00
ATOM	5200	CA	ASP	99	76.097	33.724	65.699	1.00	24.89
ATOM	5201	CB	ASP	99	76.070	33.929	67.212	1.00	23.81
ATOM	5202	CG	ASP	99	77.255	33.499	68.044	1.00	23.56
ATOM	5203	OD1	ASP	99	78.296	33.216	67.459	1.00	24.89
ATOM	5204	OD2	ASP	99	77.116	33.443	69.274	1.00	24.46
ATOM	5205	C	ASP	99	76.397	32.266	65.325	1.00	27.31
ATOM	5206	O	ASP	99	76.675	31.422	66.175	1.00	27.53

117/145

FIGURE 1 (CONT.)

ATOM	5207	N	MET	100	76.454	31.959	64.022	1.00	28.62
ATOM	5208	H	MET	100	76.263	32.694	63.401	1.00	0.00
ATOM	5209	CA	MET	100	76.682	30.597	63.526	1.00	26.59
ATOM	5210	CB	MET	100	77.091	30.731	62.098	1.00	26.12
ATOM	5211	CG	MET	100	75.785	31.000	61.402	1.00	31.98
ATOM	5212	SD	MET	100	76.010	31.405	59.660	1.00	38.98
ATOM	5213	CE	MET	100	76.583	29.831	59.099	1.00	42.31
ATOM	5214	C	MET	100	77.608	29.594	64.227	1.00	25.05
ATOM	5215	O	MET	100	77.166	28.590	64.787	1.00	24.37
ATOM	5216	N	ASP	101	78.902	29.828	64.348	1.00	25.72
ATOM	5217	H	ASP	101	79.244	30.669	63.992	1.00	0.00
ATOM	5218	CA	ASP	101	79.796	28.879	65.013	1.00	24.96
ATOM	5219	CB	ASP	101	81.206	29.256	64.642	1.00	22.87
ATOM	5220	CG	ASP	101	81.575	30.678	65.026	1.00	25.13
ATOM	5221	OD1	ASP	101	82.463	31.246	64.388	1.00	25.82
ATOM	5222	OD2	ASP	101	80.998	31.203	65.973	1.00	22.31
ATOM	5223	C	ASP	101	79.653	28.809	66.537	1.00	26.32
ATOM	5224	O	ASP	101	80.592	28.528	67.268	1.00	29.18
ATOM	5225	N	LYS	102	78.539	29.207	67.113	1.00	27.26
ATOM	5226	H	LYS	102	77.767	29.447	66.559	1.00	0.00
ATOM	5227	CA	LYS	102	78.350	29.242	68.540	1.00	27.19
ATOM	5228	CB	LYS	102	78.439	27.813	69.076	1.00	27.51
ATOM	5229	CG	LYS	102	77.554	26.775	68.350	1.00	29.02
ATOM	5230	CD	LYS	102	76.021	26.870	68.504	1.00	25.52
ATOM	5231	CE	LYS	102	75.456	25.549	67.973	1.00	24.57
ATOM	5232	NZ	LYS	102	74.903	24.699	69.015	1.00	23.47
ATOM	5233	HZ1	LYS	102	74.653	23.771	68.620	1.00	0.00
ATOM	5234	HZ2	LYS	102	74.044	25.154	69.385	1.00	0.00
ATOM	5235	HZ3	LYS	102	75.590	24.580	69.785	1.00	0.00
ATOM	5236	C	LYS	102	79.293	30.156	69.320	1.00	29.06
ATOM	5237	O	LYS	102	78.839	30.643	70.345	1.00	33.70
ATOM	5238	N	ASP	103	80.517	30.567	68.964	1.00	29.06
ATOM	5239	H	ASP	103	80.883	30.235	68.125	1.00	0.00
ATOM	5240	CA	ASP	103	81.388	31.371	69.836	1.00	28.78
ATOM	5241	CB	ASP	103	82.680	31.540	69.072	1.00	32.33
ATOM	5242	CG	ASP	103	82.821	32.599	67.985	1.00	33.75
ATOM	5243	OD1	ASP	103	83.771	32.486	67.203	1.00	37.00
ATOM	5244	OD2	ASP	103	82.020	33.526	67.906	1.00	36.62
ATOM	5245	C	ASP	103	81.121	32.710	70.568	1.00	29.40
ATOM	5246	O	ASP	103	82.051	33.319	71.121	1.00	28.70
ATOM	5247	N	GLY	104	79.902	33.258	70.608	1.00	29.83
ATOM	5248	H	GLY	104	79.165	32.702	70.282	1.00	0.00
ATOM	5249	CA	GLY	104	79.644	34.534	71.293	1.00	30.15
ATOM	5250	C	GLY	104	79.781	35.855	70.507	1.00	29.23
ATOM	5251	O	GLY	104	79.377	36.907	70.998	1.00	30.73

118/145

FIGURE 1 (CONT.)

ATOM	5252	N	TYR	105	80.311	35.889	69.286	1.00	28.10
ATOM	5253	H	TYR	105	80.593	35.038	68.902	1.00	0.00
ATOM	5254	CA	TYR	105	80.485	37.110	68.497	1.00	27.18
ATOM	5255	CB	TYR	105	81.962	37.463	68.307	1.00	27.91
ATOM	5256	CG	TYR	105	82.662	37.746	69.600	1.00	31.20
ATOM	5257	CD1	TYR	105	82.574	39.042	70.084	1.00	33.04
ATOM	5258	CE1	TYR	105	83.001	39.313	71.373	1.00	35.53
ATOM	5259	CD2	TYR	105	83.213	36.705	70.363	1.00	31.78
ATOM	5260	CE2	TYR	105	83.641	36.976	71.663	1.00	32.77
ATOM	5261	CZ	TYR	105	83.514	38.284	72.165	1.00	35.60
ATOM	5262	OH	TYR	105	83.757	38.589	73.496	1.00	35.29
ATOM	5263	HH	TYR	105	84.025	37.791	73.960	1.00	0.00
ATOM	5264	C	TYR	105	79.921	36.995	67.083	1.00	26.94
ATOM	5265	O	TYR	105	80.333	36.077	66.384	1.00	26.80
ATOM	5266	N	ILE	106	79.023	37.837	66.567	1.00	25.40
ATOM	5267	H	ILE	106	78.583	38.437	67.194	1.00	0.00
ATOM	5268	CA	ILE	106	78.561	37.816	65.172	1.00	21.05
ATOM	5269	CB	ILE	106	77.168	38.456	65.050	1.00	18.84
ATOM	5270	CG2	ILE	106	76.774	38.343	63.589	1.00	16.28
ATOM	5271	CG1	ILE	106	76.131	37.804	65.961	1.00	13.65
ATOM	5272	CD1	ILE	106	75.030	38.763	66.314	1.00	8.95
ATOM	5273	C	ILE	106	79.501	38.543	64.202	1.00	22.56
ATOM	5274	O	ILE	106	79.582	39.773	64.075	1.00	20.04
ATOM	5275	N	SER	107	80.182	37.700	63.450	1.00	22.11
ATOM	5276	H	SER	107	80.017	36.748	63.589	1.00	0.00
ATOM	5277	CA	SER	107	81.109	38.170	62.444	1.00	22.53
ATOM	5278	CB	SER	107	82.038	37.070	61.957	1.00	20.87
ATOM	5279	OG	SER	107	81.323	36.165	61.126	1.00	21.98
ATOM	5280	HG	SER	107	81.566	35.264	61.383	1.00	0.00
ATOM	5281	C	SER	107	80.370	38.666	61.228	1.00	23.39
ATOM	5282	O	SER	107	79.307	38.133	60.930	1.00	25.31
ATOM	5283	N	ASN	108	80.947	39.610	60.468	1.00	26.13
ATOM	5284	H	ASN	108	81.713	40.073	60.868	1.00	0.00
ATOM	5285	CA	ASN	108	80.413	40.103	59.176	1.00	26.33
ATOM	5286	CB	ASN	108	81.525	40.974	58.555	1.00	24.46
ATOM	5287	CG	ASN	108	81.168	41.683	57.256	1.00	29.73
ATOM	5288	OD1	ASN	108	80.364	41.233	56.441	1.00	30.26
ATOM	5289	ND2	ASN	108	81.729	42.807	56.896	1.00	27.31
ATOM	5290	HD21	ASN	108	82.394	43.273	57.425	1.00	0.00
ATOM	5291	HD22	ASN	108	81.370	43.083	56.021	1.00	0.00
ATOM	5292	C	ASN	108	79.948	38.972	58.229	1.00	26.85
ATOM	5293	O	ASN	108	78.846	38.967	57.676	1.00	27.81
ATOM	5294	N	GLY	109	80.743	37.901	58.210	1.00	26.08
ATOM	5295	H	GLY	109	81.530	37.934	58.786	1.00	0.00
ATOM	5296	CA	GLY	109	80.511	36.717	57.378	1.00	25.57

119/145

FIGURE 1 (CONT.)

ATOM	5297	C	GLY	109	79.237	35.974	57.679	1.00	26.47
ATOM	5298	O	GLY	109	78.487	35.629	56.763	1.00	29.73
ATOM	5299	N	GLU	110	78.988	35.765	58.974	1.00	26.38
ATOM	5300	H	GLU	110	79.655	36.085	59.621	1.00	0.00
ATOM	5301	CA	GLU	110	77.759	35.166	59.502	1.00	22.46
ATOM	5302	CB	GLU	110	77.819	34.952	60.921	1.00	23.04
ATOM	5303	CG	GLU	110	78.834	33.892	61.116	1.00	25.08
ATOM	5304	CD	GLU	110	79.326	33.780	62.528	1.00	26.42
ATOM	5305	OE1	GLU	110	79.206	34.755	63.275	1.00	24.76
ATOM	5306	OE2	GLU	110	79.843	32.703	62.841	1.00	29.02
ATOM	5307	C	GLU	110	76.594	36.097	59.336	1.00	24.39
ATOM	5308	O	GLU	110	75.506	35.634	58.969	1.00	23.48
ATOM	5309	N	LEU	111	76.851	37.413	59.542	1.00	22.30
ATOM	5310	H	LEU	111	77.722	37.690	59.889	1.00	0.00
ATOM	5311	CA	LEU	111	75.786	38.363	59.324	1.00	22.27
ATOM	5312	CB	LEU	111	76.193	39.809	59.646	1.00	20.27
ATOM	5313	CG	LEU	111	75.298	40.576	60.676	1.00	18.88
ATOM	5314	CD1	LEU	111	75.591	42.042	60.509	1.00	16.83
ATOM	5315	CD2	LEU	111	73.790	40.354	60.476	1.00	15.28
ATOM	5316	C	LEU	111	75.320	38.311	57.879	1.00	23.14
ATOM	5317	O	LEU	111	74.129	38.062	57.638	1.00	24.07
ATOM	5318	N	PHE	112	76.208	38.453	56.888	1.00	23.90
ATOM	5319	H	PHE	112	77.116	38.730	57.106	1.00	0.00
ATOM	5320	CA	PHE	112	75.786	38.314	55.499	1.00	23.26
ATOM	5321	CB	PHE	112	77.001	38.563	54.577	1.00	20.22
ATOM	5322	CG	PHE	112	76.625	38.492	53.090	1.00	20.57
ATOM	5323	CD1	PHE	112	76.684	37.272	52.396	1.00	17.93
ATOM	5324	CD2	PHE	112	76.202	39.635	52.426	1.00	18.72
ATOM	5325	CE1	PHE	112	76.314	37.225	51.059	1.00	20.01
ATOM	5326	CE2	PHE	112	75.836	39.569	51.083	1.00	19.54
ATOM	5327	CZ	PHE	112	75.887	38.370	50.393	1.00	18.60
ATOM	5328	C	PHE	112	75.166	36.918	55.252	1.00	24.79
ATOM	5329	O	PHE	112	74.034	36.842	54.773	1.00	26.07
ATOM	5330	N	GLN	113	75.791	35.790	55.583	1.00	24.77
ATOM	5331	H	GLN	113	76.688	35.870	55.963	1.00	0.00
ATOM	5332	CA	GLN	113	75.172	34.484	55.393	1.00	27.20
ATOM	5333	CB	GLN	113	76.102	33.455	56.031	1.00	30.75
ATOM	5334	CG	GLN	113	76.849	32.498	55.082	1.00	41.23
ATOM	5335	CD	GLN	113	77.974	33.041	54.163	1.00	47.37
ATOM	5336	OE1	GLN	113	78.070	32.719	52.971	1.00	49.20
ATOM	5337	NE2	GLN	113	78.934	33.844	54.596	1.00	47.87
ATOM	5338	HE21	GLN	113	78.923	34.151	55.521	1.00	0.00
ATOM	5339	HE22	GLN	113	79.595	34.054	53.909	1.00	0.00
ATOM	5340	C	GLN	113	73.723	34.319	55.940	1.00	26.35
ATOM	5341	O	GLN	113	72.783	33.907	55.251	1.00	26.56

120/145

FIGURE 1 (CONT.)

ATOM	5342	N	VAL	114	73.468	34.689	57.183	1.00	23.35
ATOM	5343	H	VAL	114	74.206	35.048	57.714	1.00	0.00
ATOM	5344	CA	VAL	114	72.148	34.576	57.782	1.00	24.03
ATOM	5345	CB	VAL	114	72.376	34.747	59.309	1.00	22.75
ATOM	5346	CG1	VAL	114	71.049	34.755	60.092	1.00	21.95
ATOM	5347	CG2	VAL	114	73.257	33.596	59.764	1.00	20.17
ATOM	5348	C	VAL	114	71.080	35.552	57.208	1.00	26.11
ATOM	5349	O	VAL	114	69.885	35.257	57.033	1.00	24.79
ATOM	5350	N	LEU	115	71.471	36.783	56.885	1.00	25.17
ATOM	5351	H	LEU	115	72.390	37.059	57.105	1.00	0.00
ATOM	5352	CA	LEU	115	70.536	37.692	56.257	1.00	24.36
ATOM	5353	CB	LEU	115	71.154	39.054	56.146	1.00	20.53
ATOM	5354	CG	LEU	115	71.517	39.664	57.440	1.00	16.89
ATOM	5355	CD1	LEU	115	72.199	40.949	57.068	1.00	17.86
ATOM	5356	CD2	LEU	115	70.322	39.841	58.362	1.00	16.11
ATOM	5357	C	LEU	115	70.196	37.190	54.866	1.00	26.20
ATOM	5358	O	LEU	115	69.033	37.091	54.485	1.00	27.73
ATOM	5359	N	LYS	116	71.243	36.831	54.114	1.00	28.62
ATOM	5360	H	LYS	116	72.130	36.924	54.526	1.00	0.00
ATOM	5361	CA	LYS	116	71.152	36.314	52.752	1.00	29.48
ATOM	5362	CB	LYS	116	72.539	35.834	52.374	1.00	31.44
ATOM	5363	CG	LYS	116	72.703	35.307	50.970	1.00	37.30
ATOM	5364	CD	LYS	116	74.023	34.507	50.970	1.00	42.94
ATOM	5365	CE	LYS	116	74.476	34.118	49.547	1.00	45.49
ATOM	5366	NZ	LYS	116	74.645	35.290	48.696	1.00	47.17
ATOM	5367	HZ1	LYS	116	75.356	35.926	49.109	1.00	0.00
ATOM	5368	HZ2	LYS	116	73.739	35.794	48.612	1.00	0.00
ATOM	5369	HZ3	LYS	116	74.957	34.994	47.750	1.00	0.00
ATOM	5370	C	LYS	116	70.121	35.192	52.613	1.00	28.92
ATOM	5371	O	LYS	116	69.254	35.251	51.743	1.00	27.83
ATOM	5372	N	MET	117	70.171	34.230	53.568	1.00	28.75
ATOM	5373	H	MET	117	70.908	34.288	54.214	1.00	0.00
ATOM	5374	CA	MET	117	69.274	33.071	53.626	1.00	25.77
ATOM	5375	CB	MET	117	69.756	32.049	54.623	1.00	24.82
ATOM	5376	CG	MET	117	69.583	32.128	56.127	1.00	25.63
ATOM	5377	SD	MET	117	70.092	30.532	56.857	1.00	28.13
ATOM	5378	CE	MET	117	71.867	30.610	56.986	1.00	16.67
ATOM	5379	C	MET	117	67.828	33.347	53.954	1.00	25.30
ATOM	5380	O	MET	117	66.941	32.556	53.643	1.00	26.93
ATOM	5381	N	MET	118	67.595	34.493	54.564	1.00	22.91
ATOM	5382	H	MET	118	68.351	34.989	54.937	1.00	0.00
ATOM	5383	CA	MET	118	66.252	34.967	54.760	1.00	22.57
ATOM	5384	CB	MET	118	66.037	35.670	56.092	1.00	25.13
ATOM	5385	CG	MET	118	66.079	34.897	57.408	1.00	24.54
ATOM	5386	SD	MET	118	66.018	36.098	58.769	1.00	25.16

121/145

FIGURE 1 (CONT.)

ATOM	5387	CE	MET	118	67.755	36.223	59.060	1.00	25.97
ATOM	5388	C	MET	118	65.888	35.995	53.715	1.00	23.77
ATOM	5389	O	MET	118	64.701	36.294	53.611	1.00	25.11
ATOM	5390	N	VAL	119	66.800	36.635	52.960	1.00	23.41
ATOM	5391	H	VAL	119	67.749	36.483	53.142	1.00	0.00
ATOM	5392	CA	VAL	119	66.369	37.638	51.982	1.00	24.25
ATOM	5393	CB	VAL	119	67.341	38.853	52.175	1.00	25.42
ATOM	5394	CG1	VAL	119	68.631	38.676	51.416	1.00	25.15
ATOM	5395	CG2	VAL	119	66.683	40.106	51.652	1.00	25.73
ATOM	5396	C	VAL	119	66.248	37.181	50.498	1.00	24.97
ATOM	5397	O	VAL	119	65.598	37.774	49.606	1.00	23.28
ATOM	5398	N	GLY	120	66.934	36.060	50.276	1.00	24.64
ATOM	5399	H	GLY	120	67.466	35.709	51.020	1.00	0.00
ATOM	5400	CA	GLY	120	67.008	35.385	49.003	1.00	25.51
ATOM	5401	C	GLY	120	67.590	36.309	47.958	1.00	27.72
ATOM	5402	O	GLY	120	68.688	36.861	48.107	1.00	29.69
ATOM	5403	N	ALA	121	66.800	36.539	46.907	1.00	26.98
ATOM	5404	H	ALA	121	65.935	36.089	46.869	1.00	0.00
ATOM	5405	CA	ALA	121	67.240	37.444	45.848	1.00	24.75
ATOM	5406	CB	ALA	121	67.026	36.808	44.486	1.00	24.87
ATOM	5407	C	ALA	121	66.517	38.776	45.862	1.00	24.77
ATOM	5408	O	ALA	121	66.257	39.403	44.837	1.00	26.11
ATOM	5409	N	ASN	122	66.060	39.227	47.021	1.00	24.49
ATOM	5410	H	ASN	122	66.125	38.670	47.829	1.00	0.00
ATOM	5411	CA	ASN	122	65.411	40.531	47.008	1.00	27.02
ATOM	5412	CB	ASN	122	64.306	40.528	48.033	1.00	29.77
ATOM	5413	CG	ASN	122	63.137	39.647	47.603	1.00	30.83
ATOM	5414	OD1	ASN	122	62.419	39.279	48.502	1.00	34.34
ATOM	5415	ND2	ASN	122	62.733	39.220	46.404	1.00	24.59
ATOM	5416	HD21	ASN	122	63.205	39.493	45.593	1.00	0.00
ATOM	5417	HD22	ASN	122	61.959	38.630	46.468	1.00	0.00
ATOM	5418	C	ASN	122	66.312	41.744	47.211	1.00	24.73
ATOM	5419	O	ASN	122	65.921	42.895	47.086	1.00	23.26
ATOM	5420	N	LEU	123	67.559	41.400	47.466	1.00	23.48
ATOM	5421	H	LEU	123	67.782	40.448	47.456	1.00	0.00
ATOM	5422	CA	LEU	123	68.642	42.327	47.653	1.00	25.00
ATOM	5423	CB	LEU	123	69.137	42.239	49.111	1.00	21.46
ATOM	5424	CG	LEU	123	68.840	43.139	50.310	1.00	20.78
ATOM	5425	CD1	LEU	123	69.527	44.456	50.114	1.00	20.56
ATOM	5426	CD2	LEU	123	67.364	43.383	50.479	1.00	24.04
ATOM	5427	C	LEU	123	69.764	41.885	46.673	1.00	26.76
ATOM	5428	O	LEU	123	69.943	40.686	46.416	1.00	26.82
ATOM	5429	N	LYS	124	70.466	42.801	45.986	1.00	26.51
ATOM	5430	H	LYS	124	70.064	43.686	45.881	1.00	0.00
ATOM	5431	CA	LYS	124	71.730	42.456	45.306	1.00	26.94

122/145

FIGURE 1 (CONT.)

ATOM	5432	CB	LYS	124	72.308	43.651	44.548	1.00	27.43
ATOM	5433	CG	LYS	124	71.342	44.313	43.579	1.00	28.59
ATOM	5434	CD	LYS	124	71.425	45.859	43.624	1.00	31.32
ATOM	5435	CE	LYS	124	71.448	46.587	45.017	1.00	28.42
ATOM	5436	NZ	LYS	124	70.391	46.172	45.913	1.00	22.71
ATOM	5437	HZ1	LYS	124	70.417	46.737	46.786	1.00	0.00
ATOM	5438	HZ2	LYS	124	70.496	45.162	46.133	1.00	0.00
ATOM	5439	HZ3	LYS	124	69.490	46.329	45.417	1.00	0.00
ATOM	5440	C	LYS	124	72.783	42.039	46.368	1.00	26.26
ATOM	5441	O	LYS	124	72.773	42.611	47.480	1.00	24.46
ATOM	5442	N	ASP	125	73.737	41.121	46.143	1.00	23.51
ATOM	5443	H	ASP	125	73.707	40.597	45.319	1.00	0.00
ATOM	5444	CA	ASP	125	74.631	40.788	47.243	1.00	22.27
ATOM	5445	CB	ASP	125	75.458	39.523	46.875	1.00	25.75
ATOM	5446	CG	ASP	125	74.742	38.143	47.036	1.00	31.78
ATOM	5447	OD1	ASP	125	73.764	38.015	47.779	1.00	38.34
ATOM	5448	OD2	ASP	125	75.150	37.143	46.437	1.00	33.84
ATOM	5449	C	ASP	125	75.509	41.977	47.604	1.00	21.69
ATOM	5450	O	ASP	125	75.797	42.193	48.769	1.00	24.74
ATOM	5451	N	THR	126	75.898	42.861	46.689	1.00	21.93
ATOM	5452	H	THR	126	75.812	42.593	45.755	1.00	0.00
ATOM	5453	CA	THR	126	76.608	44.122	46.995	1.00	22.45
ATOM	5454	CB	THR	126	76.903	44.862	45.683	1.00	22.69
ATOM	5455	OG1	THR	126	78.079	44.158	45.255	1.00	25.91
ATOM	5456	HG1	THR	126	78.320	44.511	44.392	1.00	0.00
ATOM	5457	CG2	THR	126	77.111	46.361	45.728	1.00	21.49
ATOM	5458	C	THR	126	75.867	45.044	47.937	1.00	22.36
ATOM	5459	O	THR	126	76.425	45.613	48.864	1.00	23.73
ATOM	5460	N	ALA	127	74.564	45.168	47.781	1.00	24.20
ATOM	5461	H	ALA	127	74.125	44.663	47.072	1.00	0.00
ATOM	5462	CA	ALA	127	73.768	45.946	48.734	1.00	26.05
ATOM	5463	CB	ALA	127	72.320	46.127	48.267	1.00	29.30
ATOM	5464	C	ALA	127	73.717	45.234	50.078	1.00	23.90
ATOM	5465	O	ALA	127	74.159	45.842	51.042	1.00	26.67
ATOM	5466	N	LEU	128	73.295	43.975	50.236	1.00	21.72
ATOM	5467	H	LEU	128	72.988	43.465	49.455	1.00	0.00
ATOM	5468	CA	LEU	128	73.376	43.343	51.554	1.00	21.95
ATOM	5469	CB	LEU	128	73.023	41.872	51.498	1.00	20.57
ATOM	5470	CG	LEU	128	72.784	41.168	52.844	1.00	17.44
ATOM	5471	CD1	LEU	128	71.685	41.813	53.677	1.00	18.03
ATOM	5472	CD2	LEU	128	72.314	39.775	52.533	1.00	18.82
ATOM	5473	C	LEU	128	74.751	43.450	52.204	1.00	23.70
ATOM	5474	O	LEU	128	74.797	43.830	53.376	1.00	27.84
ATOM	5475	N	GLN	129	75.881	43.243	51.510	1.00	21.77
ATOM	5476	H	GLN	129	75.809	42.922	50.588	1.00	0.00

123/145

FIGURE 1 (CONT.)

ATOM	5477	CA	GLN	129	77.195	43.471	52.112	1.00	21.94
ATOM	5478	CB	GLN	129	78.325	43.093	51.174	1.00	22.64
ATOM	5479	CG	GLN	129	79.715	43.171	51.843	1.00	26.48
ATOM	5480	CD	GLN	129	79.947	42.357	53.139	1.00	27.97
ATOM	5481	OE1	GLN	129	80.415	42.866	54.160	1.00	29.15
ATOM	5482	NE2	GLN	129	79.738	41.059	53.252	1.00	25.04
ATOM	5483	HE21	GLN	129	79.442	40.510	52.511	1.00	0.00
ATOM	5484	HE22	GLN	129	79.917	40.780	54.178	1.00	0.00
ATOM	5485	C	GLN	129	77.456	44.920	52.537	1.00	22.72
ATOM	5486	O	GLN	129	78.132	45.155	53.551	1.00	21.00
ATOM	5487	N	GLN	130	76.908	45.906	51.804	1.00	21.99
ATOM	5488	H	GLN	130	76.429	45.663	50.981	1.00	0.00
ATOM	5489	CA	GLN	130	77.056	47.325	52.174	1.00	19.29
ATOM	5490	CB	GLN	130	76.427	48.229	51.168	1.00	18.57
ATOM	5491	CG	GLN	130	77.360	48.359	49.975	1.00	18.83
ATOM	5492	CD	GLN	130	76.750	49.098	48.794	1.00	16.25
ATOM	5493	OE1	GLN	130	75.556	49.312	48.617	1.00	14.76
ATOM	5494	NE2	GLN	130	77.522	49.541	47.858	1.00	17.88
ATOM	5495	HE21	GLN	130	78.487	49.430	47.943	1.00	0.00
ATOM	5496	HE22	GLN	130	77.049	49.908	47.085	1.00	0.00
ATOM	5497	C	GLN	130	76.445	47.658	53.497	1.00	16.83
ATOM	5498	O	GLN	130	77.116	48.189	54.371	1.00	17.31
ATOM	5499	N	ILE	131	75.204	47.234	53.683	1.00	17.34
ATOM	5500	H	ILE	131	74.741	46.822	52.919	1.00	0.00
ATOM	5501	CA	ILE	131	74.520	47.419	54.961	1.00	16.07
ATOM	5502	CB	ILE	131	72.985	47.305	54.713	1.00	18.21
ATOM	5503	CG2	ILE	131	72.643	48.288	53.570	1.00	10.00
ATOM	5504	CG1	ILE	131	72.538	45.872	54.413	1.00	19.32
ATOM	5505	CD1	ILE	131	71.024	45.818	54.149	1.00	21.77
ATOM	5506	C	ILE	131	75.001	46.464	56.069	1.00	16.80
ATOM	5507	O	ILE	131	74.929	46.737	57.266	1.00	16.97
ATOM	5508	N	VAL	132	75.562	45.295	55.757	1.00	20.04
ATOM	5509	H	VAL	132	75.472	44.965	54.837	1.00	0.00
ATOM	5510	CA	VAL	132	76.244	44.475	56.757	1.00	17.43
ATOM	5511	CB	VAL	132	76.663	43.165	56.156	1.00	16.54
ATOM	5512	CG1	VAL	132	77.656	42.512	57.052	1.00	18.19
ATOM	5513	CG2	VAL	132	75.475	42.230	56.029	1.00	13.84
ATOM	5514	C	VAL	132	77.455	45.289	57.163	1.00	19.71
ATOM	5515	O	VAL	132	77.566	45.643	58.329	1.00	24.60
ATOM	5516	N	ASP	133	78.327	45.730	56.270	1.00	21.28
ATOM	5517	H	ASP	133	78.243	45.443	55.344	1.00	0.00
ATOM	5518	CA	ASP	133	79.437	46.577	56.676	1.00	20.22
ATOM	5519	CB	ASP	133	80.245	47.013	55.491	1.00	24.55
ATOM	5520	CG	ASP	133	80.918	45.901	54.714	1.00	25.28
ATOM	5521	CD1	ASP	133	81.603	45.076	55.302	1.00	28.10

124/145

FIGURE 1 (CONT.)

ATOM	5522	OD2	ASP	133	80.766	45.867	53.502	1.00	27.72
ATOM	5523	C	ASP	133	79.074	47.840	57.448	1.00	20.60
ATOM	5524	O	ASP	133	79.735	48.099	58.457	1.00	22.11
ATOM	5525	N	LYS	134	78.044	48.638	57.132	1.00	19.05
ATOM	5526	H	LYS	134	77.565	48.473	56.290	1.00	0.00
ATOM	5527	CA	LYS	134	77.795	49.813	57.955	1.00	16.85
ATOM	5528	CB	LYS	134	76.853	50.720	57.264	1.00	14.20
ATOM	5529	CG	LYS	134	77.506	51.297	56.012	1.00	13.44
ATOM	5530	CD	LYS	134	76.582	52.210	55.171	1.00	18.59
ATOM	5531	CE	LYS	134	76.709	51.735	53.717	1.00	19.89
ATOM	5532	NZ	LYS	134	75.946	52.516	52.776	1.00	19.69
ATOM	5533	HZ1	LYS	134	76.248	53.507	52.820	1.00	0.00
ATOM	5534	HZ2	LYS	134	74.936	52.454	53.011	1.00	0.00
ATOM	5535	HZ3	LYS	134	76.103	52.150	51.817	1.00	0.00
ATOM	5536	C	LYS	134	77.264	49.458	59.309	1.00	18.93
ATOM	5537	O	LYS	134	77.717	50.010	60.297	1.00	23.74
ATOM	5538	N	THR	135	76.449	48.402	59.435	1.00	21.95
ATOM	5539	H	THR	135	76.215	47.929	58.607	1.00	0.00
ATOM	5540	CA	THR	135	75.872	47.935	60.723	1.00	20.19
ATOM	5541	CB	THR	135	74.942	46.665	60.601	1.00	18.29
ATOM	5542	OG1	THR	135	73.734	47.074	59.954	1.00	15.58
ATOM	5543	HG1	THR	135	73.947	47.172	59.009	1.00	0.00
ATOM	5544	CG2	THR	135	74.541	46.069	61.952	1.00	16.61
ATOM	5545	C	THR	135	76.942	47.563	61.716	1.00	21.35
ATOM	5546	O	THR	135	76.856	47.769	62.923	1.00	23.55
ATOM	5547	N	ILE	136	77.986	46.949	61.199	1.00	23.01
ATOM	5548	H	ILE	136	77.968	46.688	60.251	1.00	0.00
ATOM	5549	CA	ILE	136	79.108	46.566	62.049	1.00	22.07
ATOM	5550	CB	ILE	136	79.802	45.406	61.318	1.00	16.58
ATOM	5551	CG2	ILE	136	81.171	45.192	61.857	1.00	18.53
ATOM	5552	CG1	ILE	136	78.877	44.200	61.415	1.00	13.96
ATOM	5553	CD1	ILE	136	79.432	42.881	60.976	1.00	11.84
ATOM	5554	C	ILE	136	79.970	47.809	62.286	1.00	24.21
ATOM	5555	O	ILE	136	80.316	48.103	63.422	1.00	26.21
ATOM	5556	N	ILE	137	80.208	48.676	61.307	1.00	25.73
ATOM	5557	H	ILE	137	79.864	48.475	60.412	1.00	0.00
ATOM	5558	CA	ILE	137	81.002	49.881	61.512	1.00	26.77
ATOM	5559	CB	ILE	137	81.065	50.657	60.157	1.00	29.17
ATOM	5560	CG2	ILE	137	81.584	52.090	60.319	1.00	32.32
ATOM	5561	CG1	ILE	137	81.970	49.916	59.227	1.00	27.13
ATOM	5562	CD1	ILE	137	81.801	50.473	57.816	1.00	30.89
ATOM	5563	C	ILE	137	80.399	50.739	62.621	1.00	27.48
ATOM	5564	O	ILE	137	81.083	51.353	63.431	1.00	28.74
ATOM	5565	N	ASN	138	79.078	50.742	62.704	1.00	28.53
ATOM	5566	H	ASN	138	78.559	50.260	62.027	1.00	0.00

125/145

FIGURE 1 (CONT.)

ATOM	5567	CA	ASN	138	78.433	51.574	63.700	1.00	28.82
ATOM	5568	CB	ASN	138	77.175	52.186	63.115	1.00	28.01
ATOM	5569	CG	ASN	138	77.523	53.174	62.029	1.00	29.44
ATOM	5570	OD1	ASN	138	76.931	53.157	60.969	1.00	31.71
ATOM	5571	ND2	ASN	138	78.477	54.078	62.144	1.00	31.58
ATOM	5572	HD21	ASN	138	79.024	54.144	62.946	1.00	0.00
ATOM	5573	HD22	ASN	138	78.535	54.652	61.357	1.00	0.00
ATOM	5574	C	ASN	138	78.084	50.977	65.031	1.00	27.02
ATOM	5575	O	ASN	138	77.640	51.665	65.941	1.00	29.38
ATOM	5576	N	ALA	139	78.294	49.704	65.188	1.00	27.24
ATOM	5577	H	ALA	139	78.608	49.178	64.423	1.00	0.00
ATOM	5578	CA	ALA	139	77.893	49.078	66.445	1.00	27.48
ATOM	5579	CB	ALA	139	76.752	48.071	66.155	1.00	29.87
ATOM	5580	C	ALA	139	79.035	48.385	67.146	1.00	26.61
ATOM	5581	O	ALA	139	78.986	48.018	68.308	1.00	25.14
ATOM	5582	N	ASP	140	80.102	48.214	66.385	1.00	26.29
ATOM	5583	H	ASP	140	80.026	48.430	65.433	1.00	0.00
ATOM	5584	CA	ASP	140	81.354	47.695	66.853	1.00	28.92
ATOM	5585	CB	ASP	140	82.131	47.323	65.614	1.00	30.11
ATOM	5586	CG	ASP	140	83.550	46.817	65.744	1.00	31.44
ATOM	5587	OD1	ASP	140	84.353	47.143	64.861	1.00	33.77
ATOM	5588	OD2	ASP	140	83.836	46.100	66.704	1.00	31.14
ATOM	5589	C	ASP	140	82.069	48.740	67.708	1.00	30.84
ATOM	5590	O	ASP	140	83.160	49.269	67.447	1.00	31.44
ATOM	5591	N	LYS	141	81.454	48.938	68.862	1.00	31.24
ATOM	5592	H	LYS	141	80.671	48.387	69.065	1.00	0.00
ATOM	5593	CA	LYS	141	81.891	49.906	69.844	1.00	32.18
ATOM	5594	CB	LYS	141	80.645	50.242	70.663	1.00	28.42
ATOM	5595	CG	LYS	141	79.860	51.332	69.912	1.00	25.33
ATOM	5596	CD	LYS	141	78.420	51.077	70.202	1.00	25.80
ATOM	5597	CE	LYS	141	77.577	52.338	70.218	1.00	27.06
ATOM	5598	NZ	LYS	141	77.420	52.934	68.910	1.00	29.36
ATOM	5599	HZ1	LYS	141	78.349	53.228	68.550	1.00	0.00
ATOM	5600	HZ2	LYS	141	76.785	53.754	68.978	1.00	0.00
ATOM	5601	HZ3	LYS	141	77.004	52.225	68.272	1.00	0.00
ATOM	5602	C	LYS	141	83.081	49.480	70.700	1.00	33.83
ATOM	5603	O	LYS	141	83.297	49.916	71.819	1.00	37.14
ATOM	5604	N	ASP	142	83.962	48.732	70.078	1.00	34.38
ATOM	5605	H	ASP	142	83.852	48.667	69.113	1.00	0.00
ATOM	5606	CA	ASP	142	85.114	48.118	70.680	1.00	38.14
ATOM	5607	CB	ASP	142	84.662	47.119	71.744	1.00	44.30
ATOM	5608	CG	ASP	142	85.514	45.862	71.774	1.00	49.24
ATOM	5609	OD1	ASP	142	85.004	44.826	71.336	1.00	50.65
ATOM	5610	OD2	ASP	142	86.689	45.943	72.164	1.00	55.31
ATOM	5611	C	ASP	142	85.640	47.431	69.437	1.00	38.64

126/145

FIGURE 1 (CONT.)

ATOM	5612	O	ASP	142	85.179	46.369	69.015	1.00	41.61
ATOM	5613	N	GLY	143	86.581	48.109	68.829	1.00	37.15
ATOM	5614	H	GLY	143	86.941	48.879	69.314	1.00	0.00
ATOM	5615	CA	GLY	143	87.139	47.821	67.505	1.00	34.98
ATOM	5616	C	GLY	143	87.433	46.436	66.930	1.00	33.25
ATOM	5617	O	GLY	143	88.196	46.419	65.963	1.00	34.86
ATOM	5618	N	ASP	144	86.914	45.278	67.359	1.00	31.48
ATOM	5619	H	ASP	144	86.360	45.258	68.159	1.00	0.00
ATOM	5620	CA	ASP	144	87.240	44.033	66.683	1.00	29.20
ATOM	5621	CB	ASP	144	87.109	42.897	67.669	1.00	30.85
ATOM	5622	CG	ASP	144	85.749	42.672	68.301	1.00	31.31
ATOM	5623	OD1	ASP	144	85.684	42.000	69.325	1.00	31.28
ATOM	5624	OD2	ASP	144	84.758	43.140	67.760	1.00	33.44
ATOM	5625	C	ASP	144	86.459	43.688	65.424	1.00	28.83
ATOM	5626	O	ASP	144	86.713	42.672	64.783	1.00	30.85
ATOM	5627	N	GLY	145	85.436	44.431	65.032	1.00	27.19
ATOM	5628	H	GLY	145	85.274	45.238	65.539	1.00	0.00
ATOM	5629	CA	GLY	145	84.759	44.143	63.760	1.00	26.86
ATOM	5630	C	GLY	145	83.762	42.996	63.736	1.00	27.14
ATOM	5631	O	GLY	145	83.224	42.589	62.714	1.00	26.66
ATOM	5632	N	ARG	146	83.519	42.432	64.897	1.00	28.83
ATOM	5633	H	ARG	146	84.093	42.684	65.642	1.00	0.00
ATOM	5634	CA	ARG	146	82.516	41.396	65.105	1.00	29.27
ATOM	5635	CB	ARG	146	83.278	40.085	65.388	1.00	27.24
ATOM	5636	CG	ARG	146	84.075	39.993	66.666	1.00	27.75
ATOM	5637	CD	ARG	146	84.829	38.690	66.538	1.00	33.54
ATOM	5638	NE	ARG	146	85.126	38.056	67.825	1.00	36.79
ATOM	5639	HE	ARG	146	84.507	37.382	68.167	1.00	0.00
ATOM	5640	CZ	ARG	146	86.250	38.261	68.509	1.00	37.51
ATOM	5641	NH1	ARG	146	86.421	37.656	69.678	1.00	39.08
ATOM	5642	HH11	ARG	146	85.706	37.055	70.037	1.00	0.00
ATOM	5643	HH12	ARG	146	87.265	37.800	70.194	1.00	0.00
ATOM	5644	NH2	ARG	146	87.228	39.029	68.026	1.00	41.44
ATOM	5645	HH21	ARG	146	87.136	39.454	67.125	1.00	0.00
ATOM	5646	HH22	ARG	146	88.069	39.152	68.553	1.00	0.00
ATOM	5647	C	ARG	146	81.534	41.794	66.246	1.00	29.45
ATOM	5648	O	ARG	146	81.954	42.379	67.252	1.00	33.12
ATOM	5649	N	ILE	147	80.219	41.568	66.196	1.00	27.05
ATOM	5650	H	ILE	147	79.853	41.106	65.413	1.00	0.00
ATOM	5651	CA	ILE	147	79.350	42.048	67.266	1.00	23.37
ATOM	5652	CB	ILE	147	78.032	42.505	66.619	1.00	20.25
ATOM	5653	CG2	ILE	147	77.082	43.082	67.648	1.00	20.76
ATOM	5654	CG1	ILE	147	78.341	43.548	65.539	1.00	18.36
ATOM	5655	CD1	ILE	147	79.319	44.725	65.821	1.00	13.61
ATOM	5656	C	ILE	147	79.105	41.071	68.401	1.00	24.21

127/145

FIGURE 1 (CONT.)

ATOM	5657	O	ILE	147	78.742	39.916	68.236	1.00	22.85
ATOM	5658	N	SER	148	79.376	41.511	69.629	1.00	27.21
ATOM	5659	H	SER	148	79.798	42.385	69.707	1.00	0.00
ATOM	5660	CA	SER	148	79.142	40.708	70.846	1.00	25.93
ATOM	5661	CB	SER	148	80.107	41.136	71.927	1.00	26.53
ATOM	5662	OG	SER	148	79.858	42.475	72.360	1.00	29.92
ATOM	5663	HG	SER	148	80.719	42.904	72.473	1.00	0.00
ATOM	5664	C	SER	148	77.742	40.798	71.436	1.00	24.32
ATOM	5665	O	SER	148	77.006	41.742	71.157	1.00	26.85
ATOM	5666	N	PHE	149	77.258	39.947	72.312	1.00	23.12
ATOM	5667	H	PHE	149	77.774	39.140	72.523	1.00	0.00
ATOM	5668	CA	PHE	149	75.902	40.122	72.852	1.00	24.59
ATOM	5669	CB	PHE	149	75.658	38.981	73.838	1.00	21.83
ATOM	5670	CG	PHE	149	74.232	38.862	74.283	1.00	18.19
ATOM	5671	CD1	PHE	149	73.931	39.002	75.632	1.00	23.47
ATOM	5672	CD2	PHE	149	73.242	38.669	73.337	1.00	18.74
ATOM	5673	CE1	PHE	149	72.593	38.961	76.046	1.00	22.69
ATOM	5674	CE2	PHE	149	71.917	38.629	73.733	1.00	20.23
ATOM	5675	CZ	PHE	149	71.594	38.777	75.083	1.00	24.07
ATOM	5676	C	PHE	149	75.541	41.470	73.513	1.00	27.54
ATOM	5677	O	PHE	149	74.413	41.945	73.401	1.00	27.21
ATOM	5678	N	GLU	150	76.508	42.116	74.202	1.00	32.20
ATOM	5679	H	GLU	150	77.361	41.647	74.251	1.00	0.00
ATOM	5680	CA	GLU	150	76.359	43.403	74.910	1.00	32.39
ATOM	5681	CB	GLU	150	77.673	43.736	75.663	1.00	36.29
ATOM	5682	CG	GLU	150	77.501	44.714	76.866	1.00	45.20
ATOM	5683	CD	GLU	150	78.738	45.309	77.610	1.00	49.03
ATOM	5684	OE1	GLU	150	78.846	45.174	78.842	1.00	50.92
ATOM	5685	OE2	GLU	150	79.583	45.957	76.985	1.00	50.03
ATOM	5686	C	GLU	150	76.053	44.465	73.844	1.00	32.49
ATOM	5687	O	GLU	150	75.160	45.309	73.968	1.00	34.18
ATOM	5688	N	GLU	151	76.743	44.318	72.708	1.00	30.06
ATOM	5689	H	GLU	151	77.392	43.587	72.659	1.00	0.00
ATOM	5690	CA	GLU	151	76.582	45.179	71.538	1.00	27.95
ATOM	5691	CB	GLU	151	77.722	45.024	70.655	1.00	27.41
ATOM	5692	CG	GLU	151	78.974	45.560	71.223	1.00	26.99
ATOM	5693	CD	GLU	151	80.085	45.380	70.236	1.00	26.59
ATOM	5694	OE1	GLU	151	80.079	44.421	69.458	1.00	27.15
ATOM	5695	OE2	GLU	151	80.972	46.212	70.282	1.00	31.01
ATOM	5696	C	GLU	151	75.358	44.947	70.671	1.00	27.92
ATOM	5697	O	GLU	151	74.765	45.906	70.202	1.00	30.21
ATOM	5698	N	PHE	152	75.038	43.684	70.344	1.00	25.50
ATOM	5699	H	PHE	152	75.739	43.012	70.455	1.00	0.00
ATOM	5700	CA	PHE	152	73.759	43.283	69.783	1.00	21.63
ATOM	5701	CB	PHE	152	73.720	41.779	69.829	1.00	22.89

128/145

FIGURE 1 (CONT.)

ATOM	5702	CG	PHE	152	72.399	41.129	69.437	1.00	20.92
ATOM	5703	CD1	PHE	152	71.626	40.509	70.424	1.00	18.72
ATOM	5704	CD2	PHE	152	71.983	41.131	68.095	1.00	20.98
ATOM	5705	CE1	PHE	152	70.435	39.886	70.069	1.00	17.93
ATOM	5706	CE2	PHE	152	70.792	40.507	67.744	1.00	21.29
ATOM	5707	CZ	PHE	152	70.024	39.887	68.737	1.00	20.25
ATOM	5708	C	PHE	152	72.644	43.891	70.637	1.00	21.29
ATOM	5709	O	PHE	152	71.799	44.665	70.208	1.00	20.17
ATOM	5710	N	CYS	153	72.712	43.613	71.926	1.00	20.84
ATOM	5711	H	CYS	153	73.368	42.951	72.214	1.00	0.00
ATOM	5712	CA	CYS	153	71.802	44.196	72.895	1.00	21.20
ATOM	5713	CB	CYS	153	72.170	43.733	74.276	1.00	24.94
ATOM	5714	SG	CYS	153	71.713	41.998	74.483	1.00	33.11
ATOM	5715	C	CYS	153	71.696	45.697	72.935	1.00	19.20
ATOM	5716	O	CYS	153	70.617	46.210	73.160	1.00	22.83
ATOM	5717	N	ALA	154	72.791	46.432	72.793	1.00	19.00
ATOM	5718	H	ALA	154	73.652	45.973	72.872	1.00	0.00
ATOM	5719	CA	ALA	154	72.785	47.878	72.648	1.00	15.82
ATOM	5720	CB	ALA	154	74.155	48.374	72.404	1.00	16.16
ATOM	5721	C	ALA	154	71.950	48.417	71.498	1.00	15.52
ATOM	5722	O	ALA	154	71.420	49.518	71.488	1.00	15.51
ATOM	5723	N	VAL	155	71.894	47.596	70.469	1.00	18.52
ATOM	5724	H	VAL	155	72.416	46.770	70.534	1.00	0.00
ATOM	5725	CA	VAL	155	71.172	47.871	69.225	1.00	17.99
ATOM	5726	CB	VAL	155	71.965	47.161	68.084	1.00	16.45
ATOM	5727	CG1	VAL	155	71.214	47.283	66.807	1.00	17.16
ATOM	5728	CG2	VAL	155	73.330	47.780	67.875	1.00	11.33
ATOM	5729	C	VAL	155	69.717	47.402	69.286	1.00	21.28
ATOM	5730	O	VAL	155	68.735	48.109	69.058	1.00	22.50
ATOM	5731	N	VAL	156	69.538	46.155	69.666	1.00	24.07
ATOM	5732	H	VAL	156	70.266	45.705	70.129	1.00	0.00
ATOM	5733	CA	VAL	156	68.252	45.542	69.561	1.00	25.57
ATOM	5734	CB	VAL	156	68.660	44.133	69.129	1.00	26.17
ATOM	5735	CG1	VAL	156	68.115	42.990	69.964	1.00	27.90
ATOM	5736	CG2	VAL	156	68.219	44.101	67.676	1.00	27.18
ATOM	5737	C	VAL	156	67.329	45.686	70.759	1.00	30.00
ATOM	5738	O	VAL	156	67.655	45.593	71.951	1.00	33.12
ATOM	5739	N	GLY	157	66.117	46.035	70.304	1.00	33.79
ATOM	5740	H	GLY	157	66.058	46.207	69.344	1.00	0.00
ATOM	5741	CA	GLY	157	64.924	46.329	71.116	1.00	31.89
ATOM	5742	C	GLY	157	63.636	46.240	70.286	1.00	30.99
ATOM	5743	O	GLY	157	63.611	46.477	69.069	1.00	27.08
ATOM	5744	N	GLY	158	62.634	45.808	71.081	1.00	34.53
ATOM	5745	H	GLY	158	62.886	45.728	72.022	1.00	0.00
ATOM	5746	CA	GLY	158	61.231	45.491	70.731	1.00	36.54

129/145

FIGURE 1 (CONT.)

ATOM	5747	C	GLY	158	60.684	44.030	70.842	1.00	39.33
ATOM	5748	O	GLY	158	59.901	43.668	71.721	1.00	39.57
ATOM	5749	N	LEU	159	61.172	43.118	69.982	1.00	40.34
ATOM	5750	H	LEU	159	61.961	43.412	69.487	1.00	0.00
ATOM	5751	CA	LEU	159	60.601	41.790	69.675	1.00	38.06
ATOM	5752	CB	LEU	159	61.516	41.243	68.579	1.00	40.75
ATOM	5753	CG	LEU	159	61.120	39.907	67.966	1.00	43.73
ATOM	5754	CD1	LEU	159	59.831	40.061	67.136	1.00	46.41
ATOM	5755	CD2	LEU	159	62.295	39.381	67.178	1.00	44.55
ATOM	5756	C	LEU	159	60.195	40.607	70.582	1.00	35.89
ATOM	5757	O	LEU	159	59.153	39.983	70.356	1.00	35.30
ATOM	5758	N	ASP	160	61.033	40.175	71.531	1.00	33.06
ATOM	5759	H	ASP	160	61.897	40.627	71.564	1.00	0.00
ATOM	5760	CA	ASP	160	60.810	39.090	72.483	1.00	29.19
ATOM	5761	CB	ASP	160	61.578	39.452	73.761	1.00	26.00
ATOM	5762	CG	ASP	160	61.161	40.719	74.536	1.00	25.71
ATOM	5763	OD1	ASP	160	61.451	41.837	74.115	1.00	20.07
ATOM	5764	OD2	ASP	160	60.553	40.592	75.602	1.00	26.80
ATOM	5765	C	ASP	160	59.351	38.776	72.794	1.00	30.59
ATOM	5766	O	ASP	160	58.890	37.657	72.720	1.00	31.37
ATOM	5767	N	ILE	161	58.564	39.839	72.942	1.00	33.02
ATOM	5768	H	ILE	161	59.029	40.696	72.906	1.00	0.00
ATOM	5769	CA	ILE	161	57.126	39.841	73.216	1.00	32.58
ATOM	5770	CB	ILE	161	56.651	41.350	73.220	1.00	32.12
ATOM	5771	CG2	ILE	161	57.032	41.993	74.547	1.00	29.49
ATOM	5772	CG1	ILE	161	57.291	42.177	72.088	1.00	32.98
ATOM	5773	CD1	ILE	161	56.608	42.094	70.699	1.00	33.32
ATOM	5774	C	ILE	161	56.232	38.985	72.317	1.00	34.77
ATOM	5775	O	ILE	161	55.045	38.765	72.593	1.00	37.09
ATOM	5776	N	HIS	162	56.725	38.533	71.164	1.00	35.02
ATOM	5777	H	HIS	162	57.627	38.835	70.924	1.00	0.00
ATOM	5778	CA	HIS	162	55.965	37.616	70.302	1.00	36.29
ATOM	5779	CB	HIS	162	55.836	38.218	68.880	1.00	40.48
ATOM	5780	CG	HIS	162	54.691	39.234	68.725	1.00	44.88
ATOM	5781	CD2	HIS	162	54.484	40.006	67.588	1.00	44.78
ATOM	5782	ND1	HIS	162	53.743	39.592	69.607	1.00	46.57
ATOM	5783	HD1	HIS	162	53.651	39.252	70.530	1.00	0.00
ATOM	5784	CE1	HIS	162	52.993	40.537	69.058	1.00	46.67
ATOM	5785	NE2	HIS	162	53.452	40.778	67.843	1.00	44.72
ATOM	5786	HE2	HIS	162	53.101	41.459	67.230	1.00	0.00
ATOM	5787	C	HIS	162	56.493	36.172	70.171	1.00	35.01
ATOM	5788	O	HIS	162	55.838	35.311	69.576	1.00	33.83
ATOM	5789	N	LYS	163	57.663	35.876	70.757	1.00	33.97
ATOM	5790	H	LYS	163	58.088	36.584	71.281	1.00	0.00
ATOM	5791	CA	LYS	163	58.308	34.558	70.760	1.00	32.59

130/145

FIGURE 1 (CONT.)

ATOM	5792	CB	LYS	163	59.839	34.739	70.819	1.00	30.49
ATOM	5793	CG	LYS	163	60.573	35.263	69.572	1.00	26.88
ATOM	5794	CD	LYS	163	61.790	36.039	70.072	1.00	21.67
ATOM	5795	CE	LYS	163	62.862	36.009	69.068	1.00	18.25
ATOM	5796	NZ	LYS	163	63.204	34.609	68.947	1.00	17.76
ATOM	5797	HZ1	LYS	163	63.985	34.514	68.264	1.00	0.00
ATOM	5798	HZ2	LYS	163	62.389	34.060	68.603	1.00	0.00
ATOM	5799	HZ3	LYS	163	63.502	34.242	69.873	1.00	0.00
ATOM	5800	C	LYS	163	57.871	33.655	71.924	1.00	33.37
ATOM	5801	O	LYS	163	58.708	33.051	72.580	1.00	33.07
ATOM	5802	N	LYS	164	56.580	33.543	72.251	1.00	35.22
ATOM	5803	H	LYS	164	55.934	34.005	71.681	1.00	0.00
ATOM	5804	CA	LYS	164	56.106	32.685	73.333	1.00	38.57
ATOM	5805	CB	LYS	164	55.379	33.518	74.392	1.00	37.49
ATOM	5806	CG	LYS	164	54.138	34.269	73.964	1.00	42.53
ATOM	5807	CD	LYS	164	52.997	34.316	75.009	1.00	44.45
ATOM	5808	CE	LYS	164	52.266	32.967	75.240	1.00	46.00
ATOM	5809	NZ	LYS	164	51.084	33.183	76.077	1.00	47.57
ATOM	5810	HZ1	LYS	164	51.378	33.543	77.009	1.00	0.00
ATOM	5811	HZ2	LYS	164	50.558	32.296	76.209	1.00	0.00
ATOM	5812	HZ3	LYS	164	50.460	33.887	75.632	1.00	0.00
ATOM	5813	C	LYS	164	55.190	31.515	72.910	1.00	40.59
ATOM	5814	O	LYS	164	54.225	31.654	72.146	1.00	42.71
ATOM	5815	N	MET	165	55.495	30.305	73.391	1.00	40.41
ATOM	5816	H	MET	165	56.236	30.230	74.026	1.00	0.00
ATOM	5817	CA	MET	165	54.790	29.072	73.038	1.00	37.43
ATOM	5818	CB	MET	165	55.700	27.828	72.980	1.00	37.04
ATOM	5819	CG	MET	165	56.543	27.686	71.753	1.00	37.02
ATOM	5820	SD	MET	165	55.493	28.100	70.348	1.00	36.83
ATOM	5821	CE	MET	165	56.186	29.671	69.934	1.00	38.85
ATOM	5822	C	MET	165	53.698	28.650	73.970	1.00	36.35
ATOM	5823	O	MET	165	53.962	28.401	75.151	1.00	38.21
ATOM	5824	N	VAL	166	52.463	28.529	73.503	1.00	34.39
ATOM	5825	H	VAL	166	52.252	28.886	72.618	1.00	0.00
ATOM	5826	CA	VAL	166	51.486	27.857	74.360	1.00	31.34
ATOM	5827	CB	VAL	166	50.005	28.382	74.046	1.00	29.33
ATOM	5828	CG1	VAL	166	49.857	29.784	74.646	1.00	29.16
ATOM	5829	CG2	VAL	166	49.702	28.591	72.595	1.00	29.78
ATOM	5830	C	VAL	166	51.658	26.328	74.190	1.00	30.34
ATOM	5831	O	VAL	166	51.548	25.696	73.146	1.00	30.68
ATOM	5832	N	VAL	167	52.240	25.746	75.226	1.00	32.14
ATOM	5833	H	VAL	167	52.589	26.342	75.924	1.00	0.00
ATOM	5834	CA	VAL	167	52.487	24.299	75.323	1.00	32.77
ATOM	5835	CB	VAL	167	53.798	24.001	76.086	1.00	31.39
ATOM	5836	CG1	VAL	167	54.120	22.534	75.991	1.00	27.50

131/145

**FIGURE 1 (CONT.)**

ATOM	5837	CG2	VAL	167	54.936	24.840	75.525	1.00	32.03
ATOM	5838	C	VAL	167	51.325	23.693	76.096	1.00	34.62
ATOM	5839	O	VAL	167	50.818	24.299	77.049	1.00	33.51
ATOM	5840	N	ASP	168	50.946	22.484	75.683	1.00	38.07
ATOM	5841	H	ASP	168	51.445	22.056	74.968	1.00	0.00
ATOM	5842	CA	ASP	168	49.756	21.833	76.249	1.00	41.94
ATOM	5843	CB	ASP	168	48.730	21.605	75.091	1.00	44.80
ATOM	5844	CG	ASP	168	48.444	22.859	74.240	1.00	47.71
ATOM	5845	OD1	ASP	168	49.087	23.064	73.198	1.00	46.53
ATOM	5846	OD2	ASP	168	47.580	23.644	74.644	1.00	51.45
ATOM	5847	C	ASP	168	49.988	20.519	76.999	1.00	39.97
ATOM	5848	O	ASP	168	49.580	20.378	78.158	1.00	37.61

## FK506 COORDINATES

Atom								
	Type	Residue	#	X	Y	Z	OCC	B
ATOM	5849	O	506 908	57.006	42.568	53.877	1.00	32.39
ATOM	5850	C	506 908	55.721	42.785	53.515	1.00	31.77
ATOM	5851	O1	506 908	54.818	42.061	53.809	1.00	33.81
ATOM	5852	C1	506 908	55.441	43.968	52.579	1.00	30.46
ATOM	5853	H1	506 908	54.576	44.440	53.053	1.00	0.00
ATOM	5854	C2	506 908	54.901	43.424	51.284	1.00	26.34
ATOM	5855	H3	506 908	54.501	44.271	50.747	1.00	0.00
ATOM	5856	H2	506 908	54.043	42.763	51.433	1.00	0.00
ATOM	5857	C3	506 908	56.009	42.734	50.498	1.00	26.65
ATOM	5858	H5	506 908	55.609	42.444	49.529	1.00	0.00
ATOM	5859	H4	506 908	56.246	41.774	50.964	1.00	0.00
ATOM	5860	C4	506 908	57.301	43.539	50.324	1.00	26.47
ATOM	5861	H7	506 908	57.489	43.710	49.260	1.00	0.00
ATOM	5862	H6	506 908	58.164	42.961	50.648	1.00	0.00
ATOM	5863	C5	506 908	57.335	44.869	51.050	1.00	26.33
ATOM	5864	H9	506 908	57.016	45.648	50.351	1.00	0.00
ATOM	5865	H8	506 908	58.385	45.080	51.284	1.00	0.00
ATOM	5866	N	506 908	56.487	44.987	52.276	1.00	28.84
ATOM	5867	C6	506 908	56.575	46.057	53.127	1.00	29.05
ATOM	5868	O2	506 908	55.820	46.118	54.126	1.00	24.92
ATOM	5869	C7	506 908	57.518	47.092	52.828	1.00	29.84
ATOM	5870	O3	506 908	57.399	47.792	51.799	1.00	29.45
ATOM	5871	C8	506 908	58.776	47.296	53.794	1.00	30.12
ATOM	5872	O5	506 908	59.237	48.653	53.803	1.00	28.06
ATOM	5873	H67	506 908	59.972	48.639	53.191	1.00	0.00
ATOM	5874	C9	506 908	58.568	46.879	55.311	1.00	28.47
ATOM	5875	H10	506 908	58.033	45.932	55.372	1.00	0.00

132/145

FIGURE 1 (CONT.)

ATOM	5876	C33	506	908	57.701	47.870	56.097	1.00	30.64
ATOM	5877	H39	506	908	57.575	47.587	57.141	1.00	0.00
ATOM	5878	H40	506	908	56.699	47.959	55.678	1.00	0.00
ATOM	5879	H41	506	908	58.121	48.875	56.061	1.00	0.00
ATOM	5880	C10	506	908	59.875	46.599	56.007	1.00	28.45
ATOM	5881	H12	506	908	59.692	46.253	57.023	1.00	0.00
ATOM	5882	H11	506	908	60.433	47.531	56.105	1.00	0.00
ATOM	5883	C11	506	908	60.708	45.610	55.189	1.00	29.13
ATOM	5884	H13	506	908	60.124	44.708	55.027	1.00	0.00
ATOM	5885	O6	506	908	61.920	45.333	55.880	1.00	29.99
ATOM	5886	C41	506	908	61.855	44.360	56.903	1.00	31.23
ATOM	5887	H58	506	908	61.027	43.658	56.820	1.00	0.00
ATOM	5888	H59	506	908	61.822	44.849	57.877	1.00	0.00
ATOM	5889	H60	506	908	62.757	43.763	56.888	1.00	0.00
ATOM	5890	O4	506	908	59.819	46.574	53.125	1.00	29.88
ATOM	5891	C12	506	908	61.031	46.219	53.802	1.00	29.70
ATOM	5892	H14	506	908	61.564	47.152	53.988	1.00	0.00
ATOM	5893	C13	506	908	61.922	45.377	52.799	1.00	27.30
ATOM	5894	H15	506	908	61.756	45.824	51.815	1.00	0.00
ATOM	5895	O7	506	908	63.316	45.448	53.141	1.00	25.83
ATOM	5896	C42	506	908	64.083	46.477	52.562	1.00	23.93
ATOM	5897	H61	506	908	63.983	46.504	51.474	1.00	0.00
ATOM	5898	H62	506	908	65.137	46.303	52.771	1.00	0.00
ATOM	5899	H63	506	908	63.822	47.453	52.969	1.00	0.00
ATOM	5900	C14	506	908	61.458	43.880	52.648	1.00	25.37
ATOM	5901	H17	506	908	60.404	43.898	52.356	1.00	0.00
ATOM	5902	H16	506	908	61.429	43.395	53.619	1.00	0.00
ATOM	5903	C15	506	908	62.206	42.903	51.713	1.00	24.18
ATOM	5904	H18	506	908	61.518	42.062	51.580	1.00	0.00
ATOM	5905	C34	506	908	62.425	43.409	50.268	1.00	23.52
ATOM	5906	H42	506	908	62.607	42.595	49.568	1.00	0.00
ATOM	5907	H43	506	908	63.285	44.077	50.194	1.00	0.00
ATOM	5908	H44	506	908	61.560	43.954	49.884	1.00	0.00
ATOM	5909	C16	506	908	63.484	42.279	52.346	1.00	24.84
ATOM	5910	H20	506	908	64.056	43.041	52.867	1.00	0.00
ATOM	5911	H19	506	908	64.182	41.992	51.558	1.00	0.00
ATOM	5912	C17	506	908	63.259	41.071	53.273	1.00	22.00
ATOM	5913	C35	506	908	63.210	39.698	52.605	1.00	20.86
ATOM	5914	H45	506	908	63.668	38.913	53.203	1.00	0.00
ATOM	5915	H46	506	908	63.715	39.687	51.637	1.00	0.00
ATOM	5916	H47	506	908	62.187	39.406	52.375	1.00	0.00
ATOM	5917	C18	506	908	63.140	41.323	54.598	1.00	23.11
ATOM	5918	H21	506	908	63.113	42.365	54.899	1.00	0.00
ATOM	5919	C19	506	908	63.054	40.416	55.795	1.00	22.06
ATOM	5920	H22	506	908	63.286	39.385	55.521	1.00	0.00

133/145

FIGURE 1 (CONT.)

ATOM	5921	C36	506	908	64.081	40.804	56.856	1.00	17.62
ATOM	5922	H49	506	908	63.842	40.306	57.799	1.00	0.00
ATOM	5923	H48	506	908	64.057	41.864	57.091	1.00	0.00
ATOM	5924	C37	506	908	65.480	40.426	56.448	1.00	15.36
ATOM	5925	H29	506	908	65.917	41.028	55.666	1.00	0.00
ATOM	5926	C38	506	908	66.184	39.400	56.946	1.00	14.87
ATOM	5927	H51	506	908	67.219	39.234	56.671	1.00	0.00
ATOM	5928	H50	506	908	65.787	38.674	57.642	1.00	0.00
ATOM	5929	C20	506	908	61.588	40.446	56.252	1.00	27.35
ATOM	5930	O8	506	908	61.209	41.104	57.239	1.00	27.85
ATOM	5931	C21	506	908	60.673	39.568	55.372	1.00	29.21
ATOM	5932	H24	506	908	60.886	38.543	55.625	1.00	0.00
ATOM	5933	H23	506	908	61.036	39.599	54.367	1.00	0.00
ATOM	5934	C22	506	908	59.157	39.795	55.322	1.00	30.04
ATOM	5935	H25	506	908	58.784	39.884	56.344	1.00	0.00
ATOM	5936	O9	506	908	58.608	38.580	54.834	1.00	31.55
ATOM	5937	H68	506	908	57.730	38.790	54.486	1.00	0.00
ATOM	5938	C23	506	908	58.716	40.921	54.358	1.00	29.65
ATOM	5939	H26	506	908	59.431	41.742	54.479	1.00	0.00
ATOM	5940	C39	506	908	58.818	40.537	52.863	1.00	30.32
ATOM	5941	H52	506	908	59.662	39.921	52.569	1.00	0.00
ATOM	5942	H53	506	908	58.870	41.429	52.245	1.00	0.00
ATOM	5943	H54	506	908	57.931	39.990	52.529	1.00	0.00
ATOM	5944	C24	506	908	57.313	41.440	54.729	1.00	31.11
ATOM	5945	H27	506	908	56.623	40.615	54.503	1.00	0.00
ATOM	5946	C25	506	908	57.116	41.838	56.199	1.00	30.22
ATOM	5947	C40	506	908	57.930	43.041	56.591	1.00	27.36
ATOM	5948	H55	506	908	58.327	43.569	55.735	1.00	0.00
ATOM	5949	H56	506	908	58.758	42.755	57.237	1.00	0.00
ATOM	5950	H57	506	908	57.313	43.778	57.098	1.00	0.00
ATOM	5951	C26	506	908	56.257	41.190	57.047	1.00	29.03
ATOM	5952	H28	506	908	55.642	40.397	56.634	1.00	0.00
ATOM	5953	C27	506	908	56.057	41.427	58.546	1.00	29.20
ATOM	5954	H30	506	908	56.334	42.444	58.816	1.00	0.00
ATOM	5955	C28	506	908	54.577	41.285	58.979	1.00	31.12
ATOM	5956	H32	506	908	54.163	40.368	58.549	1.00	0.00
ATOM	5957	H31	506	908	53.981	42.073	58.521	1.00	0.00
ATOM	5958	C29	506	908	54.328	41.257	60.513	1.00	31.05
ATOM	5959	H33	506	908	54.606	42.228	60.938	1.00	0.00
ATOM	5960	O10	506	908	52.926	40.974	60.723	1.00	32.76
ATOM	5961	C43	506	908	52.128	42.001	61.313	1.00	33.01
ATOM	5962	H64	506	908	52.200	42.943	60.764	1.00	0.00
ATOM	5963	H65	506	908	52.408	42.175	62.354	1.00	0.00
ATOM	5964	H66	506	908	51.075	41.714	61.296	1.00	0.00
ATOM	5965	C30	506	908	55.256	40.175	61.170	1.00	28.01

134/145

FIGURE 1 (CONT.)

ATOM	5966	H34	506	908	54.901	39.182	60.895	1.00	0.00
ATOM	5967	O11	506	908	55.282	40.173	62.571	1.00	22.17
ATOM	5968	H69	506	908	54.354	40.168	62.831	1.00	0.00
ATOM	5969	C31	506	908	56.725	40.385	60.820	1.00	29.05
ATOM	5970	H36	506	908	57.303	39.549	61.232	1.00	0.00
ATOM	5971	H35	506	908	57.115	41.270	61.327	1.00	0.00
ATOM	5972	C32	506	908	56.974	40.475	59.316	1.00	29.10
ATOM	5973	H37	506	908	58.023	40.699	59.116	1.00	0.00
ATOM	5974	H38	506	908	56.837	39.473	58.896	1.00	0.00

135/145

FIGURE 1 (CONT.)CALCIUM ION COORDINATES

Atom							
	Type	Residue #	X	Y	Z	OCC	B
ATOM	5975	CAL CAL 901	65.324	10.388	64.524	1.00	47.05
ATOM	5976	CAL CAL 902	72.311	17.145	69.723	1.00	31.70
ATOM	5977	CAL CAL 903	80.363	33.691	65.529	1.00	30.20
ATOM	5978	CAL CAL 904	82.785	44.562	68.903	1.00	26.23

FERRIC ION COORDINATE

Atom							
	Type	Residue #	X	Y	Z	OCC	B
ATOM	5979	FE FE 905	61.528	72.037	47.242	1.00	23.55

ZINC ION COORDINATE

Atom							
	Type	Residue #	X	Y	Z	OCC	B
ATOM	5980	ZN ZN 906	62.726	69.501	46.374	1.00	30.32

PHOPHATE ION COORDINATES

Atom							
	Type	Residue #	X	Y	Z	OCC	B
ATOM	5981	O1P PO4 907	61.107	68.299	48.125	1.00	37.73
ATOM	5982	P PO4 907	59.922	69.174	48.160	1.00	30.85
ATOM	5983	O2P PO4 907	58.966	68.627	47.138	1.00	35.23
ATOM	5984	O3P PO4 907	60.371	70.557	47.823	1.00	28.17
ATOM	5985	O4P PO4 907	59.294	69.129	49.519	1.00	34.45

WATER MOLECULE COORDINATES

Atom							
	Type	Residue #	X	Y	Z	OCC	B
ATOM	5986	OH2 TIP3 1	47.336	80.672	34.273	1.00	23.34
ATOM	5987	H1 TIP3 1	47.265	79.709	34.372	1.00	0.00
ATOM	5988	H2 TIP3 1	46.921	80.786	33.410	1.00	0.00
ATOM	5989	OH2 TIP3 3	71.494	62.927	28.830	1.00	16.40
ATOM	5990	H1 TIP3 3	71.733	63.680	29.374	1.00	0.00
ATOM	5991	H2 TIP3 3	70.619	62.690	29.142	1.00	0.00
ATOM	5992	OH2 TIP3 4	60.670	28.930	59.843	1.00	26.01
ATOM	5993	H1 TIP3 4	60.551	28.181	59.250	1.00	0.00
ATOM	5994	H2 TIP3 4	60.213	28.690	60.652	1.00	0.00
ATOM	5995	OH2 TIP3 5	102.239	64.992	56.010	1.00	33.43

FIGURE 1 (CONT.)

ATOM	5996	H1	TIP3	5	102.312	64.823	55.068	1.00	0.00
ATOM	5997	H2	TIP3	5	102.779	64.294	56.401	1.00	0.00
ATOM	5998	OH2	TIP3	6	85.259	82.104	37.937	1.00	23.58
ATOM	5999	H1	TIP3	6	85.871	81.703	38.558	1.00	0.00
ATOM	6000	H2	TIP3	6	84.816	82.779	38.459	1.00	0.00
ATOM	6001	OH2	TIP3	7	54.673	85.588	58.504	1.00	20.86
ATOM	6002	H1	TIP3	7	53.881	86.128	58.460	1.00	0.00
ATOM	6003	H2	TIP3	7	54.519	84.890	57.857	1.00	0.00
ATOM	6004	OH2	TIP3	8	67.239	82.097	55.155	1.00	34.16
ATOM	6005	H1	TIP3	8	67.193	82.312	56.094	1.00	0.00
ATOM	6006	H2	TIP3	8	68.160	81.883	55.004	1.00	0.00
ATOM	6007	OH2	TIP3	9	55.449	36.212	66.550	1.00	36.02
ATOM	6008	H1	TIP3	9	55.279	35.669	65.776	1.00	0.00
ATOM	6009	H2	TIP3	9	55.498	35.567	67.272	1.00	0.00
ATOM	6010	OH2	TIP3	10	76.857	57.127	53.471	1.00	28.54
ATOM	6011	H1	TIP3	10	77.389	57.371	54.232	1.00	0.00
ATOM	6012	H2	TIP3	10	77.230	57.653	52.760	1.00	0.00
ATOM	6013	OH2	TIP3	11	86.599	72.139	70.201	1.00	34.06
ATOM	6014	H1	TIP3	11	87.019	72.238	71.056	1.00	0.00
ATOM	6015	H2	TIP3	11	87.324	71.904	69.613	1.00	0.00
ATOM	6016	OH2	TIP3	12	71.575	59.398	46.514	1.00	19.65
ATOM	6017	H1	TIP3	12	71.074	59.185	47.317	1.00	0.00
ATOM	6018	H2	TIP3	12	70.891	59.346	45.826	1.00	0.00
ATOM	6019	OH2	TIP3	13	54.038	57.492	27.211	1.00	41.30
ATOM	6020	H1	TIP3	13	54.405	58.331	27.488	1.00	0.00
ATOM	6021	H2	TIP3	13	53.954	56.984	28.016	1.00	0.00
ATOM	6022	OH2	TIP3	14	82.496	86.387	58.952	1.00	24.40
ATOM	6023	H1	TIP3	14	82.026	86.463	59.787	1.00	0.00
ATOM	6024	H2	TIP3	14	81.755	86.335	58.334	1.00	0.00
ATOM	6025	OH2	TIP3	15	67.353	59.318	46.216	1.00	21.55
ATOM	6026	H1	TIP3	15	67.280	60.286	46.204	1.00	0.00
ATOM	6027	H2	TIP3	15	67.000	59.110	47.092	1.00	0.00
ATOM	6028	OH2	TIP3	16	75.668	89.508	45.560	1.00	45.41
ATOM	6029	H1	TIP3	16	76.007	90.340	45.214	1.00	0.00
ATOM	6030	H2	TIP3	16	76.407	88.905	45.432	1.00	0.00
ATOM	6031	OH2	TIP3	17	82.467	61.005	62.613	1.00	26.38
ATOM	6032	H1	TIP3	17	82.793	61.380	61.790	1.00	0.00
ATOM	6033	H2	TIP3	17	81.589	60.669	62.394	1.00	0.00
ATOM	6034	OH2	TIP3	19	59.392	90.450	30.502	1.00	27.76
ATOM	6035	H1	TIP3	19	59.469	89.491	30.423	1.00	0.00
ATOM	6036	H2	TIP3	19	59.997	90.640	31.230	1.00	0.00
ATOM	6037	OH2	TIP3	20	53.326	32.656	82.561	1.00	26.20
ATOM	6038	H1	TIP3	20	53.200	32.792	83.507	1.00	0.00
ATOM	6039	H2	TIP3	20	52.428	32.774	82.228	1.00	0.00
ATOM	6040	OH2	TIP3	21	63.402	40.149	85.242	1.00	42.97

137/145

FIGURE 1 (CONT.)

ATOM	6041	H1	TIP3	21	62.817	40.907	85.172	1.00	0.00
ATOM	6042	H2	TIP3	21	64.255	40.554	85.419	1.00	0.00
ATOM	6043	OH2	TIP3	22	64.770	35.375	81.326	1.00	18.63
ATOM	6044	H1	TIP3	22	64.285	35.235	82.148	1.00	0.00
ATOM	6045	H2	TIP3	22	65.674	35.478	81.636	1.00	0.00
ATOM	6046	OH2	TIP3	24	76.447	74.507	27.377	1.00	12.88
ATOM	6047	H1	TIP3	24	76.839	73.630	27.295	1.00	0.00
ATOM	6048	H2	TIP3	24	75.615	74.310	26.930	1.00	0.00
ATOM	6049	OH2	TIP3	25	61.766	59.700	54.342	1.00	37.89
ATOM	6050	H1	TIP3	25	61.774	59.672	55.326	1.00	0.00
ATOM	6051	H2	TIP3	25	60.891	59.331	54.181	1.00	0.00
ATOM	6052	OH2	TIP3	26	44.430	76.748	42.682	1.00	23.66
ATOM	6053	H1	TIP3	26	45.012	76.038	42.960	1.00	0.00
ATOM	6054	H2	TIP3	26	43.649	76.278	42.374	1.00	0.00
ATOM	6055	OH2	TIP3	28	83.290	62.478	38.959	1.00	20.79
ATOM	6056	H1	TIP3	28	83.774	63.127	38.444	1.00	0.00
ATOM	6057	H2	TIP3	28	83.567	62.659	39.861	1.00	0.00
ATOM	6058	OH2	TIP3	29	97.210	69.561	60.063	1.00	40.13
ATOM	6059	H1	TIP3	29	96.883	70.343	60.508	1.00	0.00
ATOM	6060	H2	TIP3	29	96.445	69.294	59.548	1.00	0.00
ATOM	6061	OH2	TIP3	30	68.288	98.497	47.783	1.00	31.72
ATOM	6062	H1	TIP3	30	69.165	98.560	48.161	1.00	0.00
ATOM	6063	H2	TIP3	30	68.430	98.184	46.891	1.00	0.00
ATOM	6064	OH2	TIP3	31	73.508	90.298	55.446	1.00	32.42
ATOM	6065	H1	TIP3	31	73.285	89.395	55.172	1.00	0.00
ATOM	6066	H2	TIP3	31	74.153	90.542	54.776	1.00	0.00
ATOM	6067	OH2	TIP3	32	48.818	41.586	57.942	1.00	19.71
ATOM	6068	H1	TIP3	32	49.303	42.308	58.367	1.00	0.00
ATOM	6069	H2	TIP3	32	48.286	41.256	58.672	1.00	0.00
ATOM	6070	OH2	TIP3	33	61.533	59.497	57.050	1.00	35.49
ATOM	6071	H1	TIP3	33	61.851	58.711	57.519	1.00	0.00
ATOM	6072	H2	TIP3	33	61.713	60.219	57.674	1.00	0.00
ATOM	6073	OH2	TIP3	34	71.997	26.621	79.347	1.00	36.22
ATOM	6074	H1	TIP3	34	72.824	26.282	79.701	1.00	0.00
ATOM	6075	H2	TIP3	34	71.648	25.877	78.847	1.00	0.00
ATOM	6076	OH2	TIP3	35	69.385	58.585	44.506	1.00	13.50
ATOM	6077	H1	TIP3	35	69.182	59.121	43.730	1.00	0.00
ATOM	6078	H2	TIP3	35	68.618	58.795	45.086	1.00	0.00
ATOM	6079	OH2	TIP3	36	66.224	81.111	17.801	1.00	27.45
ATOM	6080	H1	TIP3	36	65.543	80.610	18.261	1.00	0.00
ATOM	6081	H2	TIP3	36	66.001	82.021	18.019	1.00	0.00
ATOM	6082	OH2	TIP3	37	74.716	49.003	46.186	1.00	33.20
ATOM	6083	H1	TIP3	37	73.953	49.452	46.550	1.00	0.00
ATOM	6084	H2	TIP3	37	75.067	48.561	46.963	1.00	0.00
ATOM	6085	OH2	TIP3	38	98.702	67.424	27.542	1.00	43.66

138/145

**FIGURE 1 (CONT.)**

ATOM	6086	H1	TIP3	38	98.839	66.509	27.295	1.00	0.00
ATOM	6087	H2	TIP3	38	98.110	67.761	26.868	1.00	0.00
ATOM	6088	OH2	TIP3	39	84.094	69.567	41.374	1.00	27.40
ATOM	6089	H1	TIP3	39	84.499	68.714	41.194	1.00	0.00
ATOM	6090	H2	TIP3	39	83.608	69.753	40.567	1.00	0.00
ATOM	6091	OH2	TIP3	40	70.180	58.008	48.682	1.00	21.85
ATOM	6092	H1	TIP3	40	69.504	57.319	48.683	1.00	0.00
ATOM	6093	H2	TIP3	40	70.954	57.541	49.024	1.00	0.00
ATOM	6094	OH2	TIP3	41	55.401	51.983	36.066	1.00	34.21
ATOM	6095	H1	TIP3	41	54.937	52.813	36.166	1.00	0.00
ATOM	6096	H2	TIP3	41	54.836	51.472	35.483	1.00	0.00
ATOM	6097	OH2	TIP3	42	74.315	31.715	78.991	1.00	36.80
ATOM	6098	H1	TIP3	42	73.565	32.297	79.111	1.00	0.00
ATOM	6099	H2	TIP3	42	73.874	30.881	78.727	1.00	0.00
ATOM	6100	OH2	TIP3	43	85.548	64.644	68.987	1.00	32.11
ATOM	6101	H1	TIP3	43	85.017	63.973	69.418	1.00	0.00
ATOM	6102	H2	TIP3	43	85.450	65.412	69.553	1.00	0.00
ATOM	6103	OH2	TIP3	44	59.703	35.882	48.430	1.00	35.51
ATOM	6104	H1	TIP3	44	59.495	36.585	47.802	1.00	0.00
ATOM	6105	H2	TIP3	44	60.283	36.318	49.059	1.00	0.00
ATOM	6106	OH2	TIP3	45	69.533	30.112	73.068	1.00	19.29
ATOM	6107	H1	TIP3	45	69.460	29.151	73.037	1.00	0.00
ATOM	6108	H2	TIP3	45	70.170	30.291	72.371	1.00	0.00
ATOM	6109	OH2	TIP3	46	65.652	55.503	30.633	1.00	45.26
ATOM	6110	H1	TIP3	46	66.178	56.301	30.703	1.00	0.00
ATOM	6111	H2	TIP3	46	65.257	55.595	29.743	1.00	0.00
ATOM	6112	OH2	TIP3	47	51.206	6.734	74.457	1.00	37.94
ATOM	6113	H1	TIP3	47	51.203	6.199	73.665	1.00	0.00
ATOM	6114	H2	TIP3	47	51.988	6.455	74.933	1.00	0.00
ATOM	6115	OH2	TIP3	48	47.698	78.013	70.445	1.00	23.79
ATOM	6116	H1	TIP3	48	47.689	78.841	70.927	1.00	0.00
ATOM	6117	H2	TIP3	48	47.787	78.283	69.529	1.00	0.00
ATOM	6118	OH2	TIP3	49	99.764	74.702	51.666	1.00	35.48
ATOM	6119	H1	TIP3	49	99.927	74.946	50.754	1.00	0.00
ATOM	6120	H2	TIP3	49	98.816	74.552	51.690	1.00	0.00
ATOM	6121	OH2	TIP3	50	84.183	83.179	34.005	1.00	29.62
ATOM	6122	H1	TIP3	50	84.731	82.576	33.503	1.00	0.00
ATOM	6123	H2	TIP3	50	84.458	83.027	34.915	1.00	0.00
ATOM	6124	OH2	TIP3	51	56.439	88.980	57.676	1.00	19.78
ATOM	6125	H1	TIP3	51	56.675	89.558	58.404	1.00	0.00
ATOM	6126	H2	TIP3	51	56.251	88.141	58.111	1.00	0.00
ATOM	6127	OH2	TIP3	52	59.712	86.020	29.324	1.00	15.48
ATOM	6128	H1	TIP3	52	60.169	86.110	30.165	1.00	0.00
ATOM	6129	H2	TIP3	52	59.830	85.091	29.110	1.00	0.00
ATOM	6130	OH2	TIP3	53	101.595	65.098	51.161	1.00	29.28

139/145

FIGURE 1 (CONT.)

ATOM	6131	H1	TIP3	53	100.988	65.799	51.408	1.00	0.00
ATOM	6132	H2	TIP3	53	102.158	65.500	50.496	1.00	0.00
ATOM	6133	OH2	TIP3	54	53.851	37.912	57.213	1.00	26.35
ATOM	6134	H1	TIP3	54	54.009	37.054	56.806	1.00	0.00
ATOM	6135	H2	TIP3	54	53.176	38.292	56.646	1.00	0.00
ATOM	6136	OH2	TIP3	55	73.558	52.054	42.842	1.00	19.98
ATOM	6137	H1	TIP3	55	73.695	51.858	43.781	1.00	0.00
ATOM	6138	H2	TIP3	55	73.672	51.190	42.439	1.00	0.00
ATOM	6139	OH2	TIP3	56	87.767	64.791	40.527	1.00	26.39
ATOM	6140	H1	TIP3	56	88.462	64.141	40.419	1.00	0.00
ATOM	6141	H2	TIP3	56	88.068	65.338	41.255	1.00	0.00
ATOM	6142	OH2	TIP3	57	71.089	22.668	81.876	1.00	22.04
ATOM	6143	H1	TIP3	57	70.983	22.552	82.830	1.00	0.00
ATOM	6144	H2	TIP3	57	71.331	23.596	81.815	1.00	0.00
ATOM	6145	OH2	TIP3	58	100.862	69.035	30.631	1.00	38.85
ATOM	6146	H1	TIP3	58	100.635	68.105	30.608	1.00	0.00
ATOM	6147	H2	TIP3	58	100.492	69.373	29.815	1.00	0.00
ATOM	6148	OH2	TIP3	59	61.515	89.197	61.611	1.00	6.25
ATOM	6149	H1	TIP3	59	61.974	88.358	61.543	1.00	0.00
ATOM	6150	H2	TIP3	59	61.209	89.229	62.517	1.00	0.00
ATOM	6151	OH2	TIP3	60	81.007	61.049	38.051	1.00	16.14
ATOM	6152	H1	TIP3	60	81.397	60.192	37.880	1.00	0.00
ATOM	6153	H2	TIP3	60	81.775	61.577	38.343	1.00	0.00
ATOM	6154	OH2	TIP3	61	72.599	42.973	39.044	1.00	37.14
ATOM	6155	H1	TIP3	61	72.184	43.583	39.660	1.00	0.00
ATOM	6156	H2	TIP3	61	71.909	42.804	38.400	1.00	0.00
ATOM	6157	OH2	TIP3	62	77.614	26.247	72.486	1.00	45.60
ATOM	6158	H1	TIP3	62	78.497	25.899	72.359	1.00	0.00
ATOM	6159	H2	TIP3	62	77.052	25.650	71.987	1.00	0.00
ATOM	6160	OH2	TIP3	63	60.866	40.457	35.935	1.00	34.04
ATOM	6161	H1	TIP3	63	61.119	40.947	35.152	1.00	0.00
ATOM	6162	H2	TIP3	63	61.678	40.028	36.211	1.00	0.00
ATOM	6163	OH2	TIP3	64	94.127	73.432	48.710	1.00	57.63
ATOM	6164	H1	TIP3	64	94.313	73.250	49.633	1.00	0.00
ATOM	6165	H2	TIP3	64	93.293	73.907	48.733	1.00	0.00
ATOM	6166	OH2	TIP3	65	86.747	56.747	66.031	1.00	46.69
ATOM	6167	H1	TIP3	65	87.003	56.047	65.429	1.00	0.00
ATOM	6168	H2	TIP3	65	86.083	57.241	65.549	1.00	0.00
ATOM	6169	OH2	TIP3	66	64.991	52.254	70.196	1.00	42.84
ATOM	6170	H1	TIP3	66	65.020	51.298	70.269	1.00	0.00
ATOM	6171	H2	TIP3	66	65.902	52.519	70.326	1.00	0.00
ATOM	6172	OH2	TIP3	67	72.332	21.577	79.746	1.00	31.43
ATOM	6173	H1	TIP3	67	72.669	20.747	80.081	1.00	0.00
ATOM	6174	H2	TIP3	67	71.794	21.901	80.496	1.00	0.00
ATOM	6175	OH2	TIP3	68	56.953	90.848	29.332	1.00	29.80

140/145

FIGURE 1 (CONT.)

ATOM	6176	H1	TIP3	68	56.811	89.908	29.185	1.00	0.00
ATOM	6177	H2	TIP3	68	57.854	90.826	29.719	1.00	0.00
ATOM	6178	OH2	TIP3	69	69.360	53.403	49.577	1.00	28.09
ATOM	6179	H1	TIP3	69	68.683	52.964	49.053	1.00	0.00
ATOM	6180	H2	TIP3	69	69.156	53.064	50.465	1.00	0.00
ATOM	6181	OH2	TIP3	70	69.319	29.836	80.545	1.00	21.16
ATOM	6182	H1	TIP3	70	69.614	29.982	81.445	1.00	0.00
ATOM	6183	H2	TIP3	70	69.082	28.903	80.529	1.00	0.00
ATOM	6184	OH2	TIP3	71	51.153	76.464	56.574	1.00	27.83
ATOM	6185	H1	TIP3	71	51.959	75.941	56.522	1.00	0.00
ATOM	6186	H2	TIP3	71	51.498	77.354	56.689	1.00	0.00
ATOM	6187	OH2	TIP3	72	71.680	50.506	56.619	1.00	14.84
ATOM	6188	H1	TIP3	72	72.230	51.082	57.156	1.00	0.00
ATOM	6189	H2	TIP3	72	70.973	50.277	57.244	1.00	0.00
ATOM	6190	OH2	TIP3	73	72.642	29.649	78.390	1.00	29.75
ATOM	6191	H1	TIP3	73	71.723	29.924	78.306	1.00	0.00
ATOM	6192	H2	TIP3	73	72.543	28.726	78.670	1.00	0.00
ATOM	6193	OH2	TIP3	74	72.204	57.547	27.111	1.00	22.34
ATOM	6194	H1	TIP3	74	71.935	56.625	26.988	1.00	0.00
ATOM	6195	H2	TIP3	74	73.153	57.487	27.217	1.00	0.00
ATOM	6196	OH2	TIP3	75	68.263	22.615	73.589	1.00	17.94
ATOM	6197	H1	TIP3	75	67.446	22.413	73.123	1.00	0.00
ATOM	6198	H2	TIP3	75	68.932	22.356	72.942	1.00	0.00
ATOM	6199	OH2	TIP3	76	43.037	84.119	40.245	1.00	41.44
ATOM	6200	H1	TIP3	76	42.447	83.926	40.996	1.00	0.00
ATOM	6201	H2	TIP3	76	42.408	83.958	39.518	1.00	0.00
ATOM	6202	OH2	TIP3	77	41.149	73.038	39.924	1.00	47.77
ATOM	6203	H1	TIP3	77	41.325	72.558	39.113	1.00	0.00
ATOM	6204	H2	TIP3	77	40.323	73.492	39.755	1.00	0.00
ATOM	6205	OH2	TIP3	78	95.575	76.386	42.861	1.00	18.01
ATOM	6206	H1	TIP3	78	95.552	75.639	43.462	1.00	0.00
ATOM	6207	H2	TIP3	78	96.237	76.966	43.238	1.00	0.00
ATOM	6208	OH2	TIP3	79	68.587	58.986	35.774	1.00	23.95
ATOM	6209	H1	TIP3	79	68.116	58.193	35.488	1.00	0.00
ATOM	6210	H2	TIP3	79	67.924	59.677	35.615	1.00	0.00
ATOM	6211	OH2	TIP3	80	75.155	46.288	42.156	1.00	39.10
ATOM	6212	H1	TIP3	80	75.466	46.322	41.247	1.00	0.00
ATOM	6213	H2	TIP3	80	74.886	47.192	42.341	1.00	0.00
ATOM	6214	OH2	TIP3	81	51.611	46.003	74.162	1.00	33.51
ATOM	6215	H1	TIP3	81	51.866	46.875	73.862	1.00	0.00
ATOM	6216	H2	TIP3	81	50.656	46.036	74.216	1.00	0.00
ATOM	6217	OH2	TIP3	82	63.400	57.477	53.365	1.00	31.46
ATOM	6218	H1	TIP3	82	62.980	58.320	53.635	1.00	0.00
ATOM	6219	H2	TIP3	82	62.632	56.973	53.081	1.00	0.00
ATOM	6220	OH2	TIP3	83	84.384	73.896	65.092	1.00	28.52

141/145

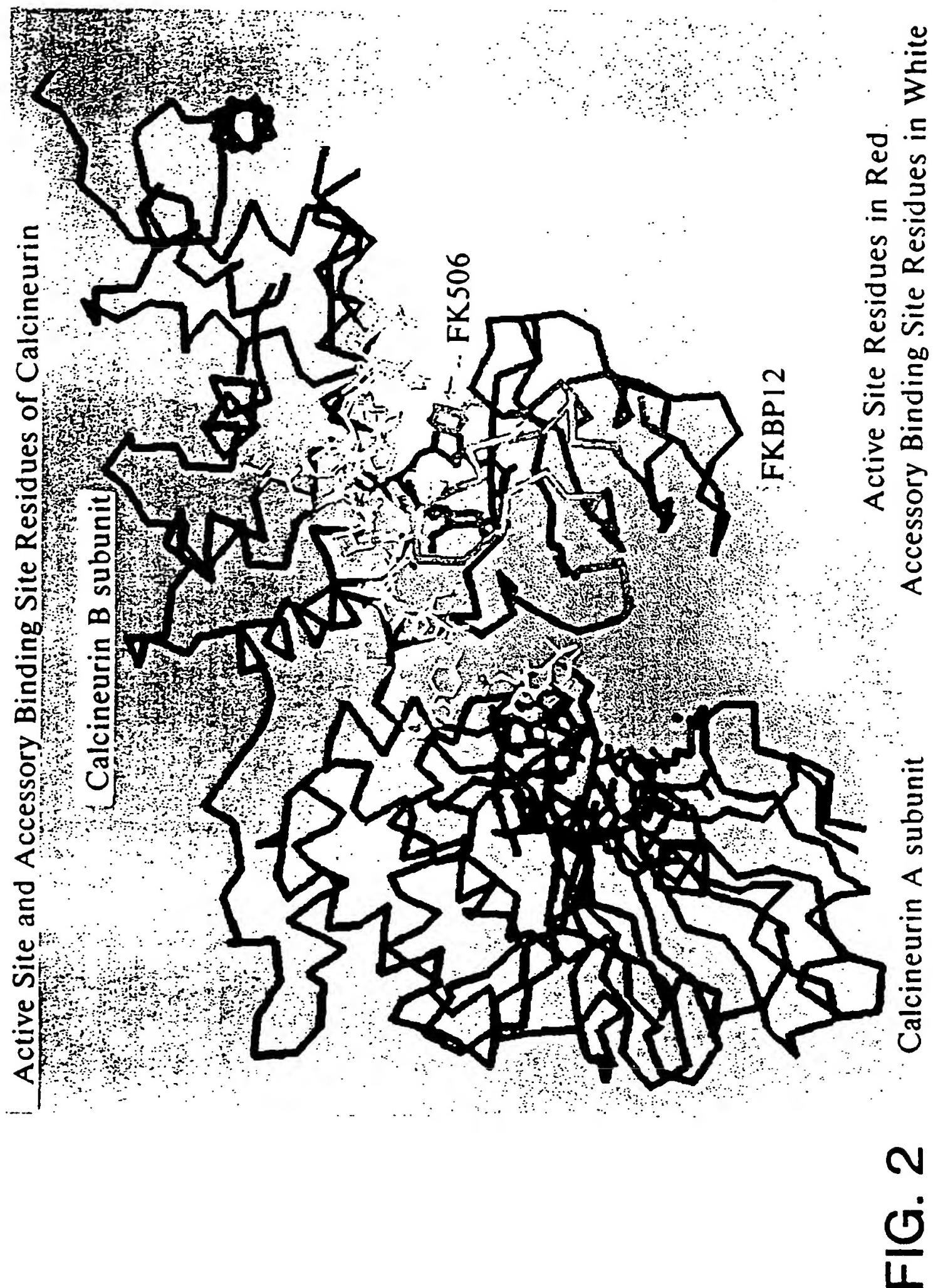
**FIGURE I (CONT.)**

ATOM	6221	H1	TIP3	83	84.574	73.410	65.896	1.00	0.00
ATOM	6222	H2	TIP3	83	84.548	74.810	65.325	1.00	0.00
ATOM	6223	OH2	TIP3	84	51.883	14.856	83.841	1.00	20.94
ATOM	6224	H1	TIP3	84	52.591	14.902	83.191	1.00	0.00
ATOM	6225	H2	TIP3	84	51.545	13.965	83.770	1.00	0.00
ATOM	6226	OH2	TIP3	85	71.836	48.721	27.742	1.00	38.58
ATOM	6227	H1	TIP3	85	72.488	48.176	28.180	1.00	0.00
ATOM	6228	H2	TIP3	85	71.250	48.091	27.319	1.00	0.00
ATOM	6229	OH2	TIP3	86	68.232	87.507	20.055	1.00	54.49
ATOM	6230	H1	TIP3	86	68.018	86.691	19.577	1.00	0.00
ATOM	6231	H2	TIP3	86	68.243	87.147	20.962	1.00	0.00
ATOM	6232	OH2	TIP3	87	68.285	31.411	75.213	1.00	31.00
ATOM	6233	H1	TIP3	87	68.779	30.910	74.528	1.00	0.00
ATOM	6234	H2	TIP3	87	68.130	32.243	74.755	1.00	0.00
ATOM	6235	OH2	TIP3	88	64.547	55.874	28.138	1.00	39.17
ATOM	6236	H1	TIP3	88	64.379	55.222	27.451	1.00	0.00
ATOM	6237	H2	TIP3	88	63.806	56.482	28.050	1.00	0.00
ATOM	6238	OH2	TIP3	89	59.857	46.342	29.666	1.00	41.24
ATOM	6239	H1	TIP3	89	59.873	45.826	28.859	1.00	0.00
ATOM	6240	H2	TIP3	89	59.300	45.838	30.258	1.00	0.00
ATOM	6241	OH2	TIP3	90	74.066	89.861	58.071	1.00	40.33
ATOM	6242	H1	TIP3	90	74.429	89.034	57.744	1.00	0.00
ATOM	6243	H2	TIP3	90	73.725	90.226	57.232	1.00	0.00
ATOM	6244	OH2	TIP3	91	78.426	56.927	35.957	1.00	25.80
ATOM	6245	H1	TIP3	91	77.517	56.670	35.781	1.00	0.00
ATOM	6246	H2	TIP3	91	78.387	57.886	35.903	1.00	0.00

142/145

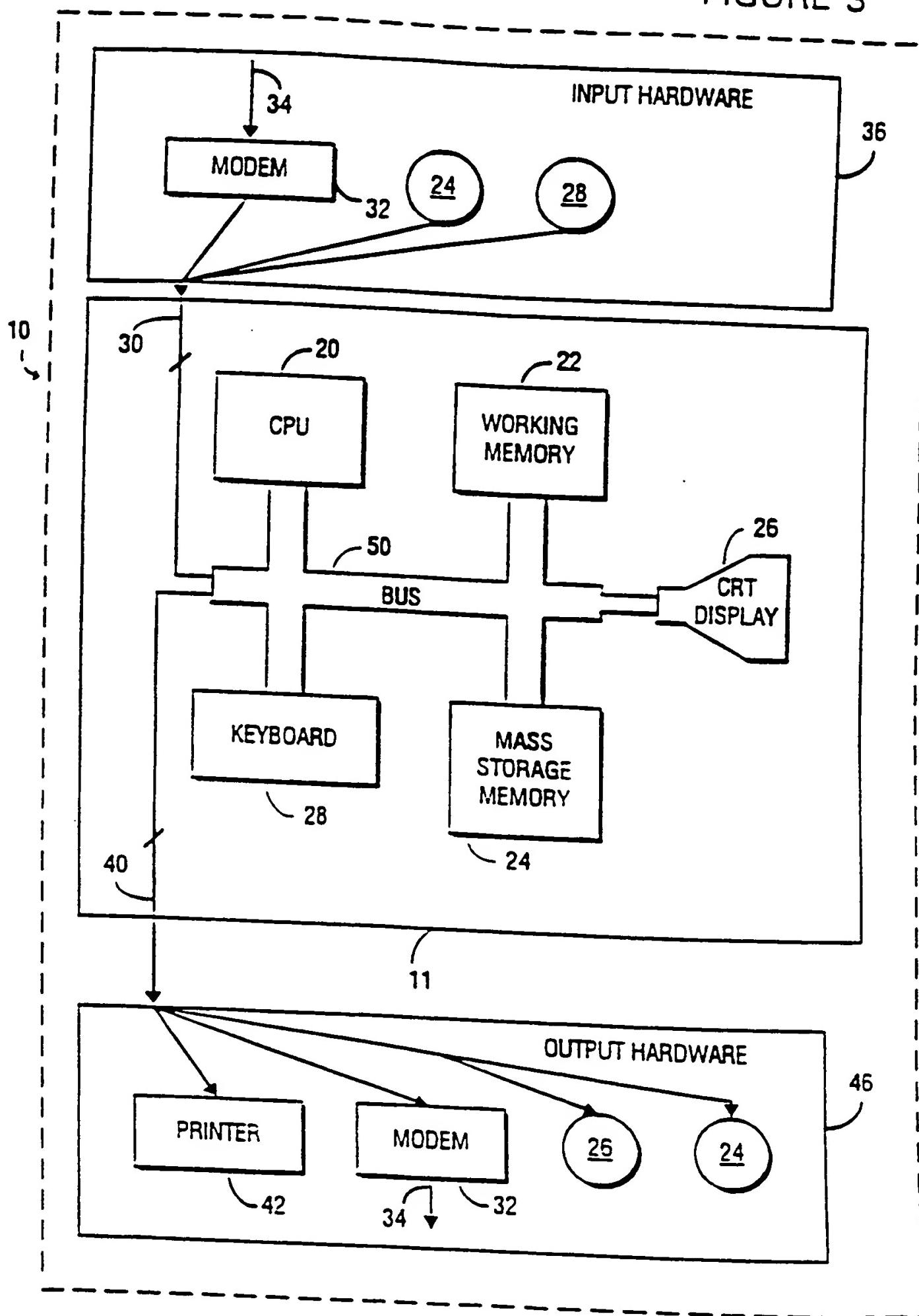
FIGURE 1 (CONT.)MYRISTATE COORDINATES

		Atom	Type	Residue #	X	Y	Z	OCC	B
ATOM	6247	CA	MYR	500	61.798	10.612	74.237	1.00	30.58
ATOM	6248	C	MYR	500	62.880	9.515	74.260	1.00	29.59
ATOM	6249	C3	MYR	500	61.342	10.943	75.657	1.00	33.83
ATOM	6250	C4	MYR	500	59.857	10.578	75.854	1.00	36.65
ATOM	6251	C5	MYR	500	59.053	11.719	76.522	1.00	36.89
ATOM	6252	C6	MYR	500	58.349	11.351	77.862	1.00	36.76
ATOM	6253	C7	MYR	500	58.416	12.451	78.960	1.00	33.84
ATOM	6254	C8	MYR	500	57.432	12.222	80.114	1.00	29.21
ATOM	6255	C9	MYR	500	57.749	13.185	81.256	1.00	26.86
ATOM	6256	C10	MYR	500	56.668	13.397	82.334	1.00	22.32
ATOM	6257	C11	MYR	500	57.032	14.557	83.258	1.00	20.60
ATOM	6258	C12	MYR	500	58.395	14.314	83.870	1.00	20.64
ATOM	6259	C13	MYR	500	59.209	15.557	84.220	1.00	25.12
ATOM	6260	C14	MYR	500	58.677	16.418	85.390	1.00	23.56



144/145.

FIGURE 3



SUBSTITUTE SHEET (RULE 26)

145/145

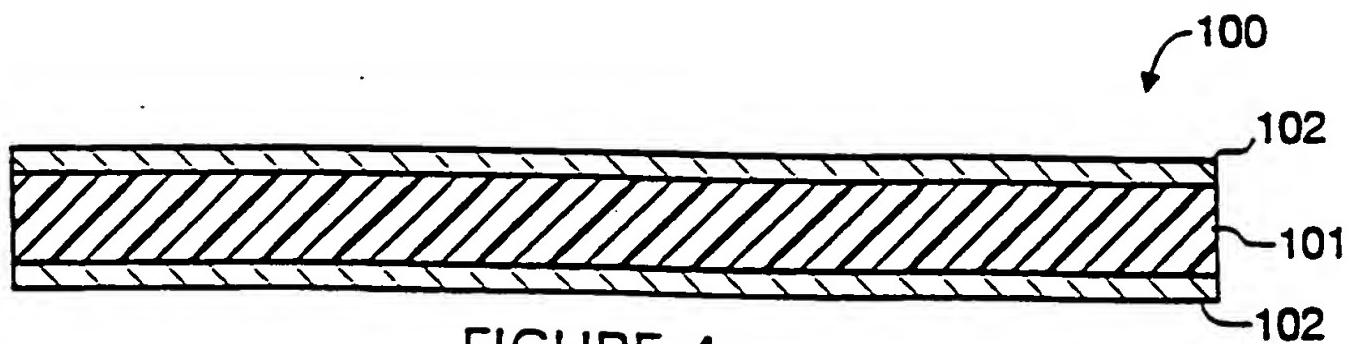


FIGURE 4

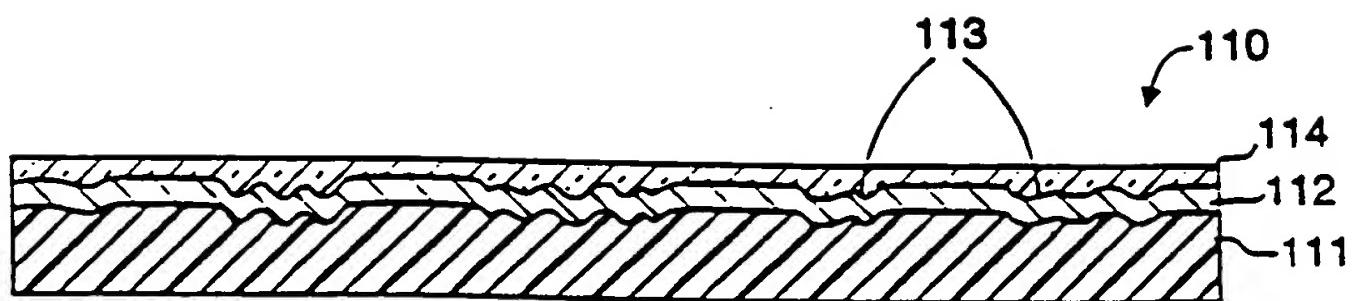


FIGURE 5

**THIS PAGE BLANK (USPTO)**



PCT

**WORLD INTELLECTUAL PROPERTY ORGANIZATION**  
International Bureau

INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification <sup>6</sup> : <b>C12N 9/16, C12P 21/06, G06F 17/50</b>		A3	(11) International Publication Number: <b>WO 97/06246</b> (43) International Publication Date: <b>20 February 1997 (20.02.97)</b>
(21) International Application Number: <b>PCT/US96/12818</b>			(81) Designated States: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, ARIPO patent (KE, LS, MW, SD, SZ, UG), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).
(22) International Filing Date: <b>1 August 1996 (01.08.96)</b>			
(30) Priority Data: 08/512,815                    9 August 1995 (09.08.95)                    US			
(71) Applicant: <b>VERTEX PHARMACEUTICALS INCORPORATED [US/US]; 130 Waverly Street, Cambridge, MA 02139-4242 (US).</b>			<b>Published</b> <i>With international search report. Before the expiration of the time limit for amending the claims and to be republished in the event of the receipt of amendments.</i>
(72) Inventors: <b>ARMISTEAD, David, M.; Five Cutting Drive, Maynard, MA 01754 (US). FITZGIBBON, Matthew, James; 163 Exchange Street, Millis, MA 02054 (US). FLEMING, Mark, Andrew; 413 Cardinal Medeiros Avenue, Cambridge, MA 02141 (US). GRIFFITH, James, P.; 15 Wood Ridge Circle, Weston, MA 02193 (US). KIM, Eunice, E.; 1500 Worcester Road, Framingham, MA 01701 (US). KIM, Joseph, L.; 20 Ridge Avenue, Natick, MA 01760 (US). SINTCHAK, Michael, D.; 34 Lloyd Street, Winchester, MA 01890 (US). THOMSON, John, Allan; 105 Slade Street, Belmont, MA 02178 (US). WILSON, Keith, P.; 6 Longwood Drive, Hopkinton, MA 01748 (US).</b>			(88) Date of publication of the international search report: <b>13 March 1997 (13.03.97)</b>
(74) Agents: <b>HALEY, James, F., Jr. et al.; Fish &amp; Neave, 1251 Avenue of the Americas, New York, NY 10020-1104 (US).</b>			

(54) Title: MOLECULES COMPRISING A CALCINEURIN-LIKE BINDING POCKET AND ENCODED DATA STORAGE MEDIUM CAPABLE OF GRAPHICALLY DISPLAYING THEM

**(57) Abstract**

The present invention relates to crystallized molecules and molecular complexes which comprise the active site binding pocket or the FKBP12/FK506 binding pocket of calcineurin or close structural homologues to either binding pocket. This invention also relates to a data storage material encoded with the corresponding structure coordinates of those crystallized molecules or molecular complexes. Such data storage material is capable of displaying such molecules and molecular complexes as a graphical three-dimensional representation on a computer screen. In addition, this invention relates to methods of using the structure coordinates of those molecules or molecular complexes to solve the structure of homologous proteins. This invention also relates to methods of using the structure coordinates to screen and design compounds that bind to calcineurin or homologues thereof.

**FOR THE PURPOSES OF INFORMATION ONLY**

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AM	Armenia	GB	United Kingdom	MW	Malawi
AT	Austria	GE	Georgia	MX	Mexico
AU	Australia	GN	Guinea	NE	Niger
BB	Barbados	GR	Greece	NL	Netherlands
BE	Belgium	HU	Hungary	NO	Norway
BF	Burkina Faso	IE	Ireland	NZ	New Zealand
BG	Bulgaria	IT	Italy	PL	Poland
BJ	Benin	JP	Japan	PT	Portugal
BR	Brazil	KE	Kenya	RO	Romania
BY	Belarus	KG	Kyrgyzstan	RU	Russian Federation
CA	Canada	KP	Democratic People's Republic of Korea	SD	Sudan
CF	Central African Republic	KR	Republic of Korea	SE	Sweden
CG	Congo	KZ	Kazakhstan	SG	Singapore
CH	Switzerland	LI	Liechtenstein	SI	Slovenia
CI	Côte d'Ivoire	LK	Sri Lanka	SK	Slovakia
CM	Cameroon	LR	Liberia	SN	Senegal
CN	China	LT	Lithuania	SZ	Swaziland
CS	Czechoslovakia	LU	Luxembourg	TD	Chad
CZ	Czech Republic	LV	Latvia	TG	Togo
DE	Germany	MC	Monaco	TJ	Tajikistan
DK	Denmark	MD	Republic of Moldova	TT	Trinidad and Tobago
EE	Estonia	MG	Madagascar	UA	Ukraine
ES	Spain	ML	Mali	UG	Uganda
FI	Finnland	MN	Mongolia	US	United States of America
FR	France	MR	Mauritania	UZ	Uzbekistan
GA	Gabon			VN	Viet Nam

# INTERNATIONAL SEARCH REPORT

International Application No

PCT/US 96/12818

**A. CLASSIFICATION OF SUBJECT MATTER**

IPC 6 C12N9/16 C12P21/06 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

**B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols)

IPC 6 C12N C12P G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	J.MOL.BIOL., vol. 235, no. 2, 1994, pages 763-768, XP000616128 D.BARFORD E.A.: "Cocrystallization of the catalytic subunit of the serine/threonine specific PP1 from human in complex with microcystin LR" see the whole document ---	1,2,7,8, 13
Y	WO,A,94 25860 (IMMUNEX CORP) 10 November 1994 see the whole document ---	14,15
Y	US,A,5 353 236 (SUBBIAH SUBRAMANIAN) 4 October 1994 see the whole document ---	14,15
Y	US,A,5 353 236 (SUBBIAH SUBRAMANIAN) 4 October 1994 see the whole document ---	14,15
		-/-

Further documents are listed in the continuation of box C.

Patent family members are listed in annex.

\* Special categories of cited documents :

- 'A' document defining the general state of the art which is not considered to be of particular relevance
- 'E' earlier document but published on or after the international filing date
- 'L' document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- 'O' document referring to an oral disclosure, use, exhibition or other means
- 'P' document published prior to the international filing date but later than the priority date claimed

- 'T' later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- 'X' document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- 'Y' document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
- '&' document member of the same patent family

3

Date of the actual completion of the international search

23 January 1997

Date of mailing of the international search report

03.02.97

Name and mailing address of the ISA

European Patent Office, P.B. 5818 Patentiaan 2  
NL - 2280 HV Rijswijk  
Tel. (+ 31-70) 340-2040, Tx. 31 651 epo nl,  
Fax (+ 31-70) 340-3016

Authorized officer

Groenendijk, M

## INTERNATIONAL SEARCH REPORT

International Application No  
PCT/us 96/12818

## C(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	CELL, vol. 82, no. 3, 11 August 1995, NA US, pages 507-522, XP002023480 J.M.GRIFFITH E.A.: "X-ray structure of calcineurin inhibited by the immunophilin-immunosuppressant FKBP12-FK506 complex" see the whole document ---	1-18
P,X	NATURE, vol. 378, 7 December 1995, LONDON GB, pages 641-644, XP002023481 C.R.KISSINGER E.A.: "Crystal structures of human calcineurin and the human FKBP12-FK506-calcineurin complex" see the whole document ---	1-18
A	BIOCHEMISTRY, vol. 28, no. 4, 1989, EASTON, PA US, pages 1868-1874, XP002023482 M.J.HUBBARD E.A.: "Functional domain structure of calcineurin A: mapping by limited proteolysis" cited in the application see the whole document ---	16-18
A	PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF USA, vol. 86, December 1989, WASHINGTON US, pages 9183-9187, XP002023483 D.GUERINI E.A.: "Cloning of human calcineurin A..." cited in the application see the whole document ---	1-18
A	SCIENCE, vol. 268, - 9 June 1995 LANCASTER, PA US, pages 1489-1492, XP002023505 N.STRÄTER E.A.: "Crystal structure of a purple acid phosphatase containing a dinuclear Fe(III)-Zn(II) active site" see the whole document ---	1-15
T	CURRENT OPINION IN BIOTECHN., vol. 7, August 1996, pages 387-402, XP000616057 J.E.VILLAFRANCA E.A.: "protein serine/threonine phosphatase" See especially page 399, column 2, paragraph 1 -----	1-15

**INTERNATIONAL SEARCH REPORT**

International application No.

PCT/US 96/12818

**Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)**

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1.  Claims Nos.: **7-12**

because they relate to subject matter not required to be searched by this Authority, namely:

**Remark:** Although claims 7-12 are directed to representation of information on a carrier, the search has been carried out as far as possible and based on the molecular structure represented by this information (Art. 17; Rule 39.1 PCT)

2.  Claims Nos.:

because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:

3.  Claims Nos.:

because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

**Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)**

This International Searching Authority found multiple inventions in this international application, as follows:

1.  As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.

2.  As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3.  As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

4.  No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

**Remark on Protest**

- The additional search fees were accompanied by the applicant's protest.
- No protest accompanied the payment of additional search fees.

**INTERNATIONAL SEARCH REPORT**

In relation on patent family members

International Application No

PCT/US 96/12818

Patent document cited in search report	Publication date	Patent family member(s)		Publication date
WO-A-9425860	10-11-94	US-A-	5453937	26-09-95
		AU-A-	6779994	21-11-94
		US-A-	5557535	17-09-96
-----	-----	-----	-----	-----
US-A-5353236	04-10-94	WO-A-	9322740	11-11-93
-----	-----	-----	-----	-----